



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 06:30 AM GMT

PDB ID : 2PF4
Title : Crystal structure of the full-length simian virus 40 small t antigen complexed with the protein phosphatase 2A Aalpha subunit
Authors : Cho, U.; Morrone, S.; Xu, W.
Deposited on : 2007-04-03
Resolution : 3.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

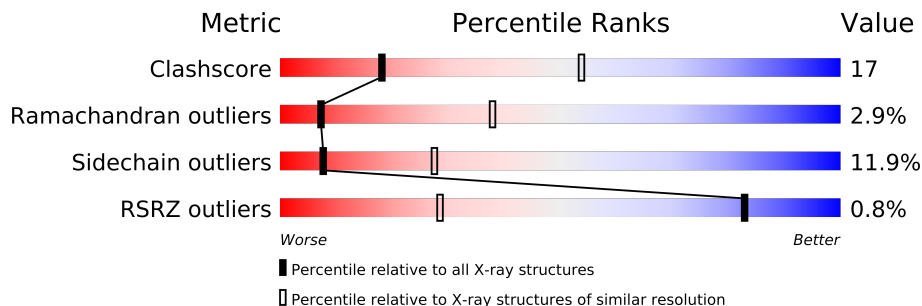
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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))
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	589	
1	B	589	
1	C	589	
1	D	589	
2	E	174	
2	F	174	
2	G	174	
2	H	174	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22802 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Serine/threonine-proteinphosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	575	Total	C	N	O	S	0	0	0
			4472	2840	754	851	27			
1	B	575	Total	C	N	O	S	0	0	0
			4473	2840	754	852	27			
1	C	577	Total	C	N	O	S	0	0	0
			4486	2849	756	854	27			
1	D	577	Total	C	N	O	S	0	0	0
			4492	2852	759	854	27			

- Molecule 2 is a protein called Small T antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	163	Total	C	N	O	S	0	0	0
			1303	836	220	227	20			
2	F	152	Total	C	N	O	S	0	0	0
			1232	790	209	213	20			
2	G	142	Total	C	N	O	S	0	0	0
			1164	748	195	201	20			
2	H	143	Total	C	N	O	S	0	0	0
			1172	751	199	202	20			

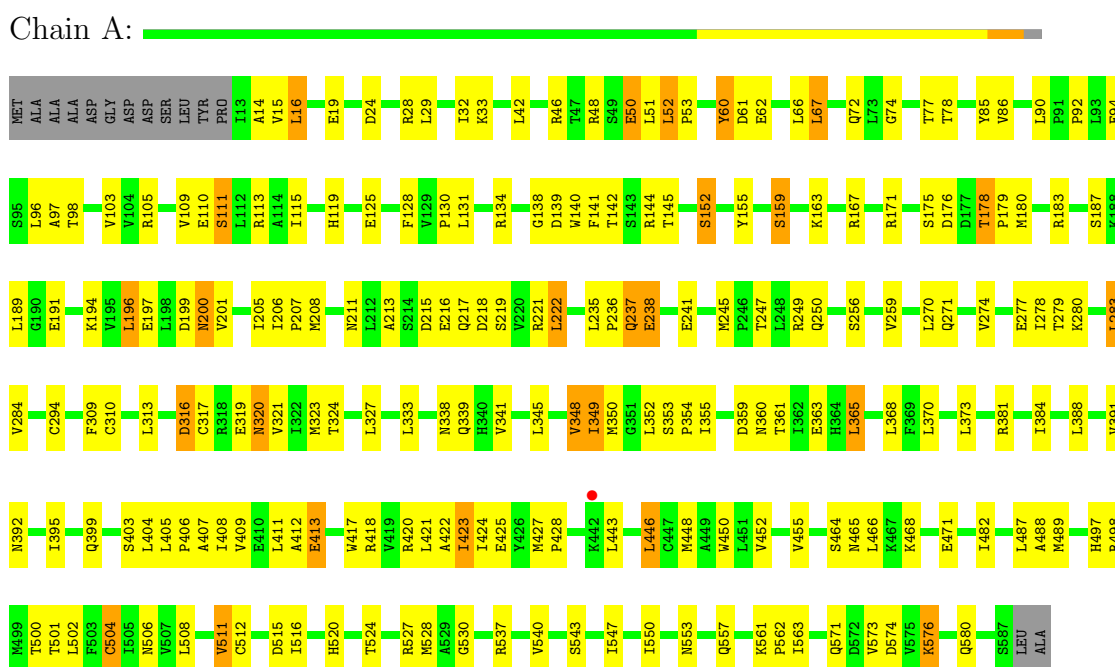
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	2	Total	Zn	0	0
			2	2		
3	G	2	Total	Zn	0	0
			2	2		
3	F	2	Total	Zn	0	0
			2	2		
3	E	2	Total	Zn	0	0
			2	2		

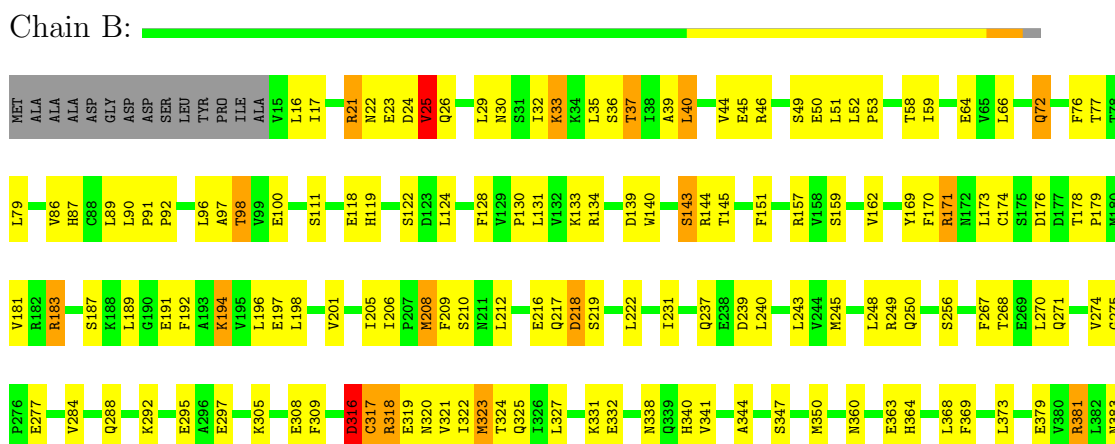
3 Residue-property plots

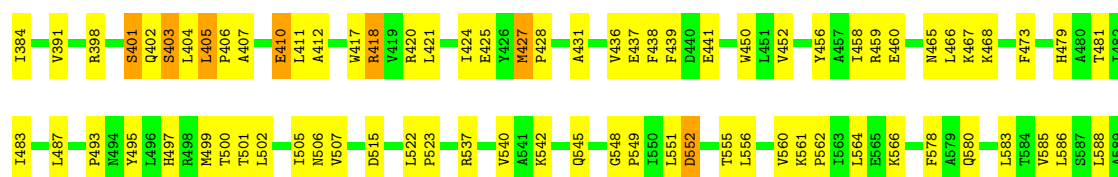
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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: Serine/threonine-proteinphosphatase 2A 65 kDa regulatory subunit A alpha isoform



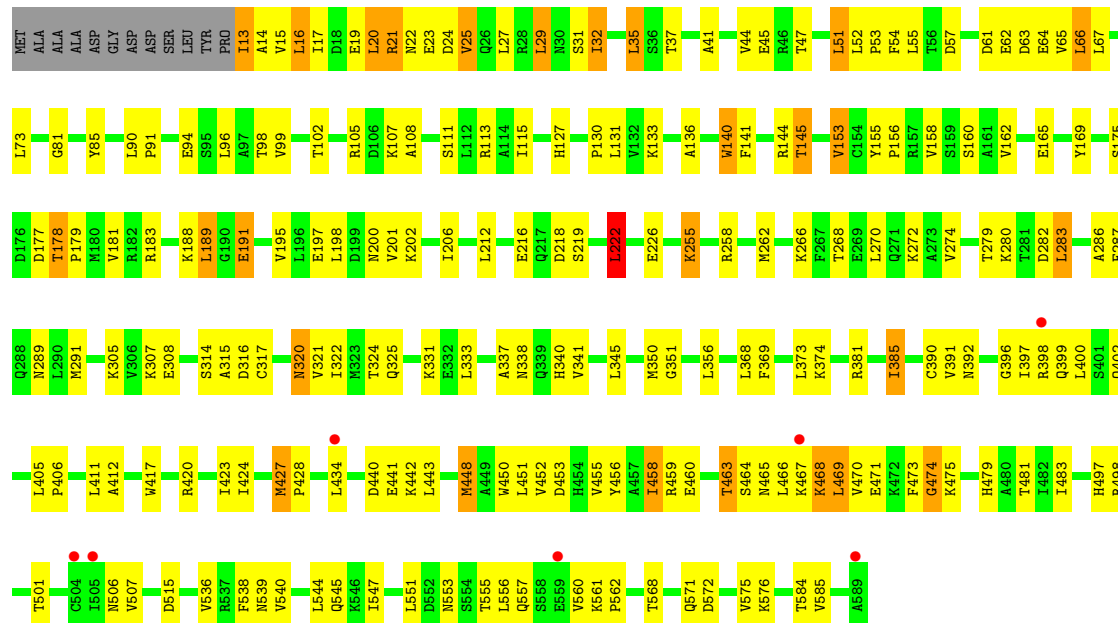
- Molecule 1: Serine/threonine-proteinphosphatase 2A 65 kDa regulatory subunit A alpha isoform





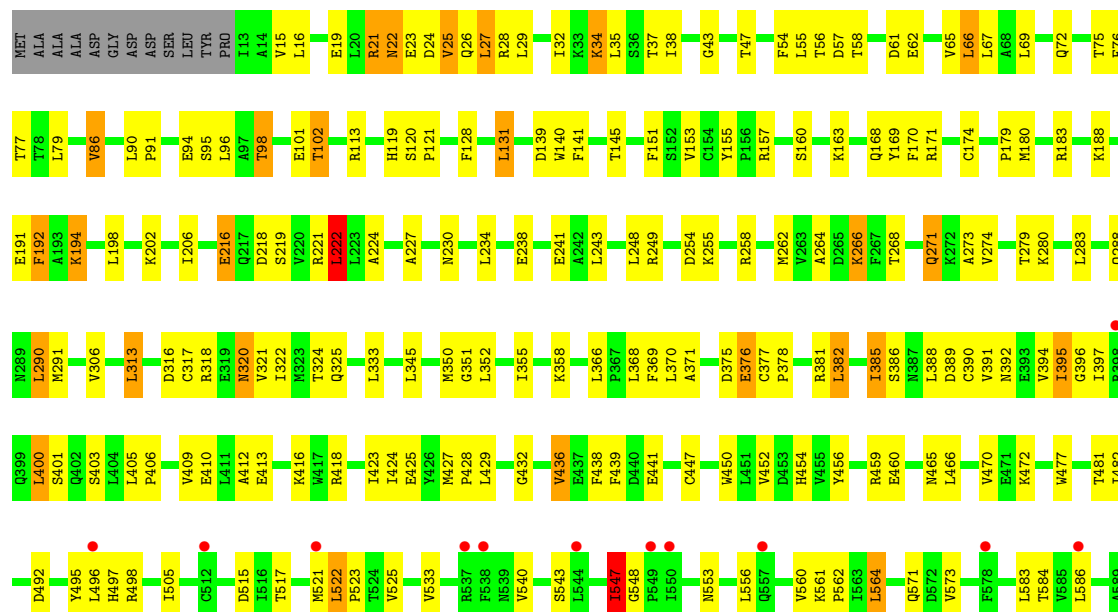
- Molecule 1: Serine/threonine-proteinphosphatase 2A 65 kDa regulatory subunit A alpha isoform

Chain C:



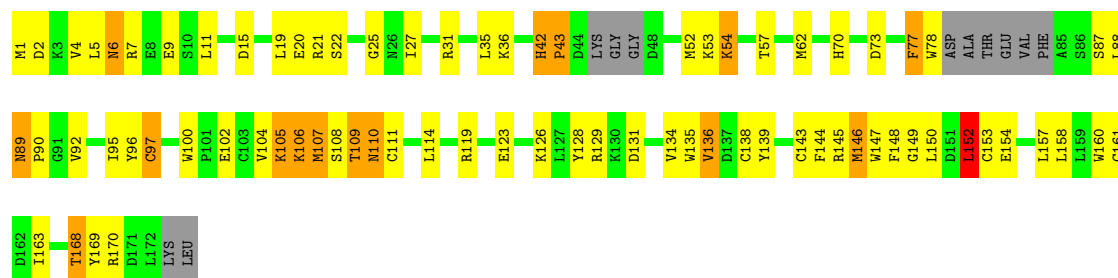
- Molecule 1: Serine/threonine-proteinphosphatase 2A 65 kDa regulatory subunit A alpha isoform

Chain D:



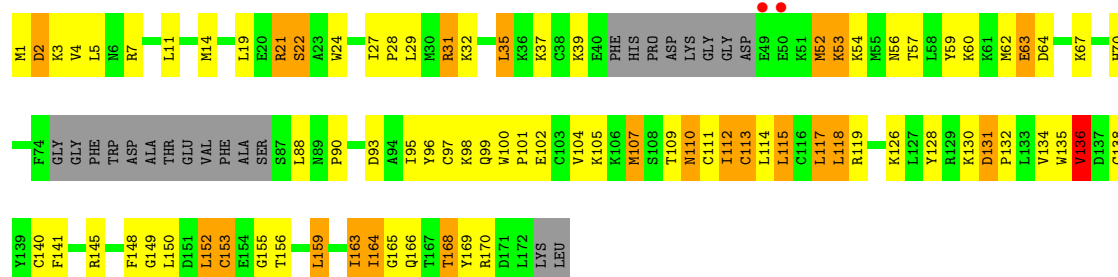
- Molecule 2: Small T antigen

Chain E:



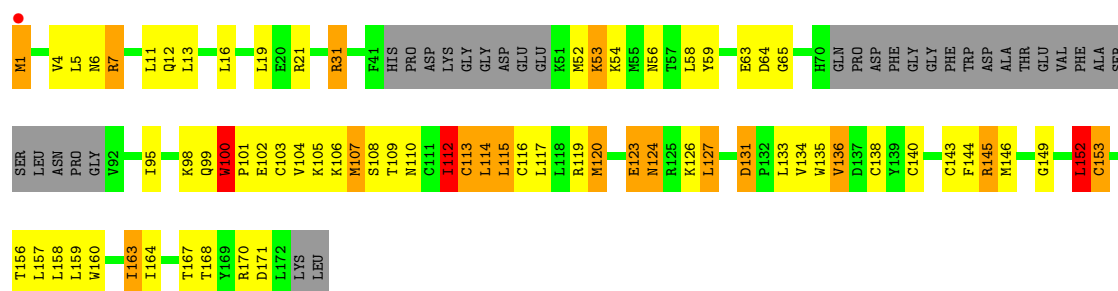
- Molecule 2: Small T antigen

Chain F:



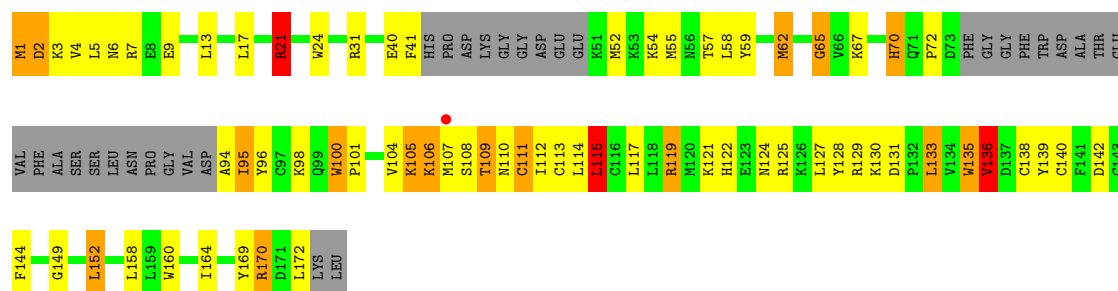
- Molecule 2: Small T antigen

Chain G:



- Molecule 2: Small T antigen

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	94.71Å 105.50Å 111.94Å 115.64° 109.55° 94.11°	Depositor
Resolution (Å)	20.00 – 3.10 47.13 – 3.11	Depositor EDS
% Data completeness (in resolution range)	97.4 (20.00-3.10) 87.3 (47.13-3.11)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.244 , 0.304 0.240 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	100.1	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 121.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 60312 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22802	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.46	0/4544	0.63	0/6170
1	B	0.50	0/4545	0.65	1/6170 (0.0%)
1	C	0.44	0/4558	0.61	2/6188 (0.0%)
1	D	0.44	0/4564	0.64	3/6195 (0.0%)
2	E	0.56	0/1332	0.73	0/1793
2	F	0.53	0/1257	0.77	0/1688
2	G	0.43	0/1186	0.71	2/1590 (0.1%)
2	H	0.49	0/1195	0.79	3/1602 (0.2%)
All	All	0.47	0/23181	0.66	11/31396 (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	B	0	2
1	D	0	2
2	E	0	1
2	H	0	1
All	All	0	6

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	115	LEU	CA-CB-CG	8.12	133.97	115.30
1	D	222	LEU	CA-CB-CG	7.28	132.04	115.30
1	D	313	LEU	CA-CB-CG	7.11	131.65	115.30
1	C	29	LEU	CA-CB-CG	6.63	130.55	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	133	LEU	CA-CB-CG	6.47	130.18	115.30
1	B	222	LEU	CA-CB-CG	6.05	129.21	115.30
1	C	222	LEU	CA-CB-CG	5.97	129.03	115.30
2	H	117	LEU	CA-CB-CG	5.83	128.71	115.30
2	G	115	LEU	CA-CB-CG	5.53	128.03	115.30
1	D	66	LEU	CA-CB-CG	5.29	127.47	115.30
2	H	133	LEU	CA-CB-CG	5.08	127.00	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	171	ARG	Sidechain
1	B	183	ARG	Sidechain
1	D	22	ASN	Peptide
1	D	436	VAL	Peptide
2	E	108	SER	Peptide
2	H	135	TRP	Peptide

5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4472	0	4567	140	0
1	B	4473	0	4567	178	0
1	C	4486	0	4583	145	0
1	D	4492	0	4594	133	0
2	E	1303	0	1265	60	0
2	F	1232	0	1222	94	0
2	G	1164	0	1168	43	0
2	H	1172	0	1170	60	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	22802	0	23136	779	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (779) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:31:ARG:HB3	2:F:31:ARG:NH1	1.70	1.07
1:D:24:ASP:HB2	1:D:28:ARG:HH21	1.23	1.03
1:D:24:ASP:HB2	1:D:28:ARG:NH2	1.77	0.99
1:B:405:LEU:HB2	1:B:406:PRO:HD3	1.45	0.99
1:B:456:TYR:HB2	2:H:128:TYR:O	1.64	0.97
1:B:183:ARG:HD3	1:B:219:SER:OG	1.64	0.97
1:B:140:TRP:NE1	2:F:131:ASP:HB3	1.79	0.96
2:H:96:TYR:O	2:H:113:CYS:HB2	1.67	0.95
1:B:421:LEU:HD23	1:D:21:ARG:HH12	1.32	0.92
1:A:16:LEU:O	1:A:19:GLU:HG2	1.71	0.91
1:B:194:LYS:HB3	1:B:194:LYS:HZ2	1.37	0.90
1:A:422:ALA:HB2	1:C:21:ARG:HD3	1.54	0.89
1:A:339:GLN:HB2	2:F:88:LEU:HD13	1.52	0.88
1:D:22:ASN:HB2	1:D:23:GLU:O	1.73	0.87
1:A:338:ASN:HD22	1:A:341:VAL:HG23	1.39	0.87
1:B:194:LYS:NZ	1:B:194:LYS:HB3	1.87	0.87
1:C:255:LYS:H	1:C:255:LYS:HE2	1.41	0.86
1:D:35:LEU:HD21	1:D:55:LEU:HD21	1.59	0.85
2:F:31:ARG:HB3	2:F:31:ARG:HH11	1.37	0.84
1:A:423:ILE:HD13	1:A:423:ILE:H	1.42	0.84
1:C:337:ALA:HB1	2:H:31:ARG:HH21	1.43	0.83
2:F:19:LEU:HD21	2:F:29:LEU:HG	1.59	0.83
1:D:24:ASP:CB	1:D:28:ARG:HH21	1.92	0.83
1:D:492:ASP:OD1	1:D:497:HIS:HB2	1.79	0.83
1:B:133:LYS:HG2	1:B:169:TYR:CE1	2.14	0.81
1:C:321:VAL:HA	1:C:324:THR:HG22	1.62	0.81
1:D:405:LEU:HB3	1:D:406:PRO:HD3	1.61	0.80
1:D:477:TRP:CZ3	1:D:482:ILE:HD11	2.17	0.80
1:D:428:PRO:HD3	1:D:465:ASN:ND2	1.97	0.80
2:F:100:TRP:O	2:F:104:VAL:HG23	1.81	0.80
1:C:13:ILE:HG12	1:C:14:ALA:H	1.45	0.79
2:H:135:TRP:CG	2:H:135:TRP:O	2.33	0.79
1:D:128:PHE:O	1:D:131:LEU:HB3	1.83	0.79
1:B:418:ARG:HG3	1:D:21:ARG:HH11	1.47	0.78
1:B:331:LYS:HG2	1:B:368:LEU:HD21	1.65	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:100:TRP:HB3	2:G:101:PRO:HD3	1.67	0.77
2:F:11:LEU:HG	2:F:21:ARG:HD2	1.66	0.77
1:C:141:PHE:O	1:C:145:THR:HG23	1.85	0.77
2:H:170:ARG:N	2:H:170:ARG:HD2	1.99	0.76
2:G:158:LEU:HB2	2:H:158:LEU:HD21	1.67	0.76
2:H:112:ILE:O	2:H:112:ILE:HG22	1.84	0.76
1:C:411:LEU:HD12	1:C:423:ILE:HD11	1.67	0.76
1:B:456:TYR:CE1	2:H:130:LYS:HD2	2.20	0.76
1:B:59:ILE:HG22	1:B:66:LEU:HD21	1.68	0.75
1:A:320:ASN:O	1:A:324:THR:HG22	1.87	0.75
1:C:411:LEU:CD1	1:C:423:ILE:HD11	2.17	0.75
1:C:412:ALA:HB1	1:C:450:TRP:HE1	1.51	0.74
1:A:94:GLU:OE1	1:A:134:ARG:NH2	2.21	0.74
1:D:454:HIS:HD2	2:F:128:TYR:HE1	1.34	0.74
1:A:109:VAL:O	1:A:113:ARG:HG3	1.88	0.74
2:E:15:ASP:OD1	2:E:21:ARG:NH2	2.20	0.73
2:E:104:VAL:HG11	2:E:152:LEU:HD21	1.70	0.73
1:B:140:TRP:HE1	2:F:131:ASP:HB3	1.53	0.73
1:A:52:LEU:HD12	1:A:92:PRO:HG3	1.70	0.73
1:B:405:LEU:HB2	1:B:406:PRO:CD	2.17	0.72
1:A:24:ASP:CG	1:A:61:ASP:HB3	2.10	0.72
1:C:470:VAL:HG13	1:C:473:PHE:O	1.90	0.72
1:B:171:ARG:HH21	1:B:171:ARG:HB2	1.53	0.72
1:B:456:TYR:HD2	1:B:459:ARG:HH22	1.36	0.72
1:B:179:PRO:HB2	1:B:183:ARG:HH21	1.54	0.72
2:G:98:LYS:O	2:G:103:CYS:SG	2.47	0.72
2:F:163:ILE:HD13	2:F:163:ILE:C	2.09	0.71
1:B:402:GLN:HG3	1:B:405:LEU:HD21	1.72	0.71
1:B:320:ASN:O	1:B:324:THR:HG22	1.90	0.71
1:B:134:ARG:HG3	1:B:134:ARG:HH21	1.53	0.71
2:E:96:TYR:CD2	2:E:161:CYS:HB2	2.26	0.71
2:F:100:TRP:HB2	2:F:101:PRO:HD3	1.73	0.71
2:F:163:ILE:HD13	2:F:163:ILE:O	1.91	0.71
2:E:168:THR:HG23	2:E:170:ARG:HE	1.55	0.71
1:C:338:ASN:HD22	1:C:341:VAL:HG23	1.56	0.71
1:A:219:SER:HB3	2:E:149:GLY:HA3	1.74	0.70
2:E:95:ILE:HG22	2:E:97:CYS:O	1.91	0.70
1:B:59:ILE:HG22	1:B:66:LEU:CD2	2.23	0.69
2:G:102:GLU:HB3	2:G:106:LYS:HE2	1.74	0.69
1:A:277:GLU:HG2	1:A:280:LYS:HE2	1.74	0.69
1:D:428:PRO:HD3	1:D:465:ASN:HD21	1.57	0.69
1:B:373:LEU:HD13	1:B:384:ILE:HG21	1.73	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:418:ARG:NH1	1:C:21:ARG:HH21	1.91	0.69
1:B:179:PRO:HB2	1:B:183:ARG:NH2	2.06	0.68
1:D:396:GLY:O	1:D:400:LEU:HB2	1.93	0.68
1:B:21:ARG:HH21	1:D:418:ARG:HD3	1.58	0.68
1:A:388:LEU:O	1:A:392:ASN:HB2	1.93	0.68
1:C:291:MET:HB3	1:C:333:LEU:HD11	1.75	0.68
1:C:197:GLU:HG2	1:C:200:ASN:HD22	1.59	0.68
2:H:1:MET:N	2:H:136:VAL:HG22	2.08	0.68
2:H:121:LYS:O	2:H:125:ARG:HB3	1.94	0.68
1:D:454:HIS:CD2	2:F:128:TYR:HE1	2.12	0.67
1:C:427:MET:N	1:C:428:PRO:HD2	2.08	0.67
1:C:314:SER:C	1:C:316:ASP:H	1.96	0.67
1:B:421:LEU:O	1:B:425:GLU:HG3	1.94	0.67
2:F:31:ARG:HB3	2:F:31:ARG:CZ	2.23	0.67
2:G:164:ILE:HA	2:G:167:THR:HG22	1.75	0.67
1:A:24:ASP:OD2	1:A:61:ASP:HB3	1.95	0.67
1:A:373:LEU:HD21	1:A:404:LEU:HD22	1.76	0.67
2:E:1:MET:HB2	2:E:136:VAL:HG22	1.77	0.66
2:H:2:ASP:CG	2:H:2:ASP:O	2.33	0.66
2:H:169:TYR:HD1	2:H:172:LEU:HA	1.59	0.66
1:A:310:CYS:HA	1:A:313:LEU:HD12	1.77	0.66
1:B:22:ASN:C	1:B:24:ASP:H	1.98	0.66
1:B:338:ASN:HD22	1:B:341:VAL:H	1.41	0.66
1:D:378:PRO:O	1:D:382:LEU:HB2	1.96	0.66
1:B:403:SER:H	1:B:405:LEU:HG	1.61	0.66
2:G:113:CYS:HB2	2:G:116:CYS:HB2	1.79	0.65
1:B:437:GLU:HG2	1:B:438:PHE:H	1.61	0.65
1:A:561:LYS:HB3	1:A:562:PRO:HD3	1.79	0.65
1:D:366:LEU:HD13	1:D:395:ILE:HD12	1.78	0.65
1:D:98:THR:CG2	1:D:140:TRP:HZ3	2.09	0.65
1:C:324:THR:HG23	1:C:325:GLN:HG2	1.77	0.65
1:D:98:THR:HG23	1:D:140:TRP:HZ3	1.61	0.65
1:C:538:PHE:HB3	1:C:575:VAL:HA	1.79	0.65
2:G:11:LEU:HD22	2:G:21:ARG:HD2	1.77	0.65
1:D:151:PHE:HB3	1:D:192:PHE:CE1	2.32	0.65
1:B:179:PRO:HB3	1:B:217:GLN:NE2	2.12	0.65
1:B:216:GLU:HB2	2:F:22:SER:HB3	1.79	0.64
2:E:105:LYS:O	2:E:107:MET:N	2.31	0.64
2:H:135:TRP:O	2:H:136:VAL:HG13	1.98	0.64
1:B:98:THR:HG23	1:B:143:SER:OG	1.98	0.64
1:C:545:GLN:HE21	1:C:585:VAL:HG21	1.60	0.64
2:F:110:ASN:HB2	2:G:110:ASN:O	1.97	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:217:GLN:HG2	1:B:219:SER:HB3	1.79	0.64
1:B:427:MET:HB3	1:B:428:PRO:HD3	1.78	0.63
1:C:162:VAL:HA	1:C:165:GLU:OE2	1.98	0.63
2:H:54:LYS:HA	2:H:57:THR:HG22	1.81	0.63
2:G:4:VAL:HG13	2:G:65:GLY:HA3	1.81	0.63
1:B:26:GLN:NE2	1:B:30:ASN:HD21	1.97	0.63
2:F:109:THR:HG22	2:F:119:ARG:HH22	1.62	0.63
1:A:60:TYR:HA	1:A:66:LEU:HD21	1.80	0.63
1:B:72:GLN:HG3	1:B:76:PHE:HE2	1.64	0.63
1:C:412:ALA:HB1	1:C:450:TRP:NE1	2.15	0.62
2:F:159:LEU:O	2:F:163:ILE:HG22	1.98	0.62
2:F:110:ASN:HD21	2:G:112:ILE:HG12	1.63	0.62
1:D:69:LEU:HD22	1:D:96:LEU:HD11	1.80	0.62
1:A:217:GLN:HE22	2:E:148:PHE:HA	1.63	0.62
1:A:152:SER:HB3	1:A:191:GLU:OE2	2.00	0.62
1:D:452:VAL:HG23	1:D:496:LEU:HB3	1.81	0.62
1:D:522:LEU:HB3	1:D:523:PRO:HD3	1.81	0.62
1:C:556:LEU:HD23	1:C:560:VAL:HG21	1.80	0.62
2:F:153:CYS:SG	2:F:155:GLY:N	2.71	0.62
2:F:150:LEU:HD13	2:F:156:THR:HG23	1.81	0.61
1:B:218:ASP:N	1:B:218:ASP:OD2	2.34	0.61
1:A:98:THR:CG2	1:A:140:TRP:HE3	2.12	0.61
1:D:98:THR:HG23	1:D:140:TRP:CZ3	2.36	0.61
1:B:456:TYR:HE1	2:H:130:LYS:HD2	1.63	0.61
1:A:391:VAL:HG12	1:A:395:ILE:HG12	1.82	0.61
2:H:4:VAL:O	2:H:5:LEU:HB2	2.01	0.61
1:D:454:HIS:O	2:F:128:TYR:HD1	1.82	0.61
2:G:131:ASP:OD1	2:G:131:ASP:N	2.30	0.61
1:B:456:TYR:CE1	2:H:130:LYS:HB2	2.36	0.61
2:F:96:TYR:O	2:F:115:LEU:HG	2.00	0.61
1:C:23:GLU:O	1:C:23:GLU:HG2	1.99	0.61
1:A:178:THR:HG23	2:E:2:ASP:CB	2.31	0.60
1:B:248:LEU:HD11	1:B:270:LEU:HD22	1.82	0.60
2:F:14:MET:HE1	2:F:24:TRP:HE3	1.66	0.60
1:B:421:LEU:HD23	1:D:21:ARG:NH1	2.10	0.60
2:F:56:ASN:O	2:F:60:LYS:HB2	2.01	0.60
1:B:467:LYS:HB2	1:B:507:VAL:HG12	1.82	0.60
1:B:548:GLY:HA2	1:B:551:LEU:HD12	1.81	0.60
1:A:411:LEU:HB3	1:A:423:ILE:HD12	1.84	0.60
1:B:317:CYS:O	1:B:317:CYS:SG	2.60	0.60
2:E:135:TRP:CZ3	2:E:144:PHE:HB2	2.36	0.60
2:F:96:TYR:OH	2:F:165:GLY:HA2	2.02	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:424:ILE:HD12	1:C:458:ILE:HG12	1.84	0.60
1:B:267:PHE:HA	1:B:270:LEU:HD12	1.83	0.60
1:B:405:LEU:CB	1:B:406:PRO:HD3	2.24	0.60
1:A:218:ASP:HA	1:A:221:ARG:HB2	1.83	0.60
1:D:227:ALA:HA	1:D:230:ASN:HD22	1.67	0.59
1:A:33:LYS:N	1:A:33:LYS:HD2	2.16	0.59
1:B:288:GLN:HE22	1:B:325:GLN:HE21	1.50	0.59
1:D:391:VAL:HG12	1:D:395:ILE:HG13	1.85	0.59
1:C:572:ASP:HB3	1:C:575:VAL:HB	1.83	0.59
2:E:6:ASN:ND2	2:E:9:GLU:OE1	2.35	0.59
2:H:144:PHE:CE1	2:H:160:TRP:HB2	2.37	0.59
1:B:379:GLU:O	1:B:383:ASN:HB2	2.02	0.59
1:D:556:LEU:HA	1:D:560:VAL:HB	1.84	0.59
1:B:324:THR:HG23	1:B:325:GLN:HG2	1.83	0.59
1:B:288:GLN:HE22	1:B:325:GLN:NE2	2.00	0.59
1:B:483:ILE:O	1:B:487:LEU:HG	2.02	0.59
1:C:268:THR:HG21	1:C:308:GLU:HB2	1.83	0.59
1:A:216:GLU:CD	1:A:216:GLU:H	2.06	0.59
2:F:1:MET:HE3	2:F:27:ILE:HD11	1.85	0.59
1:B:32:ILE:O	1:B:35:LEU:HB2	2.03	0.59
2:F:112:ILE:HA	2:F:117:LEU:HD11	1.84	0.58
1:A:553:ASN:O	1:A:557:GLN:HG2	2.03	0.58
1:D:427:MET:HE2	1:D:450:TRP:HH2	1.69	0.58
1:D:427:MET:HB3	1:D:465:ASN:HD21	1.68	0.58
1:A:294:CYS:HB2	2:F:32:LYS:HG3	1.86	0.58
1:A:500:THR:O	1:A:504:CYS:HB2	2.04	0.58
1:A:350:MET:HB3	1:A:391:VAL:HG21	1.84	0.58
2:H:1:MET:H1	2:H:136:VAL:HG22	1.68	0.57
1:C:465:ASN:O	1:C:469:LEU:HB2	2.04	0.57
1:B:17:ILE:HG22	1:D:429:LEU:HD13	1.86	0.57
1:A:216:GLU:HB3	2:E:22:SER:HA	1.86	0.57
1:A:427:MET:HB3	1:A:465:ASN:HD21	1.68	0.57
1:A:90:LEU:HB3	1:A:131:LEU:HD12	1.85	0.57
1:D:279:THR:HA	1:D:283:LEU:HB2	1.84	0.57
1:A:183:ARG:NH1	2:E:146:MET:O	2.36	0.57
2:F:96:TYR:OH	2:F:165:GLY:CA	2.52	0.57
1:D:427:MET:CE	1:D:450:TRP:HH2	2.17	0.57
1:A:213:ALA:HB1	1:A:247:THR:HG23	1.86	0.57
1:C:47:THR:HG23	1:C:51:LEU:HD11	1.86	0.57
2:H:95:ILE:CG2	2:H:113:CYS:HA	2.34	0.57
1:D:101:GLU:OE1	1:D:102:THR:N	2.37	0.57
2:H:105:LYS:HD3	2:H:152:LEU:HD21	1.85	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:136:VAL:O	2:F:136:VAL:CG2	2.52	0.57
1:B:219:SER:HB2	2:F:149:GLY:HA3	1.85	0.57
2:F:21:ARG:O	2:F:22:SER:CB	2.52	0.57
1:B:350:MET:SD	1:B:369:PHE:HB2	2.45	0.56
1:B:21:ARG:NH2	1:D:418:ARG:HD3	2.19	0.56
1:D:183:ARG:HH22	2:H:149:GLY:HA2	1.70	0.56
2:F:96:TYR:HA	2:F:114:LEU:HB2	1.86	0.56
2:H:100:TRP:HB3	2:H:101:PRO:HD3	1.85	0.56
1:C:337:ALA:HB1	2:H:31:ARG:NH2	2.17	0.56
2:F:53:LYS:HD3	2:F:54:LYS:N	2.20	0.56
1:C:451:LEU:O	1:C:459:ARG:HG3	2.04	0.56
2:H:169:TYR:C	2:H:170:ARG:HD2	2.26	0.56
1:D:548:GLY:HA3	1:D:586:LEU:HD22	1.87	0.56
1:C:155:TYR:O	1:C:158:VAL:HG22	2.05	0.56
1:B:274:VAL:HG23	1:B:275:GLY:H	1.71	0.56
1:B:46:ARG:HA	1:B:49:SER:HG	1.71	0.56
1:B:179:PRO:CB	1:B:217:GLN:NE2	2.67	0.56
1:B:46:ARG:HA	1:B:49:SER:OG	2.06	0.56
1:B:144:ARG:HH11	1:B:144:ARG:HG3	1.69	0.56
1:A:141:PHE:O	1:A:145:THR:HG23	2.06	0.56
1:A:349:ILE:HG23	1:A:350:MET:HG2	1.86	0.56
1:C:350:MET:SD	1:C:391:VAL:HG21	2.46	0.56
2:F:88:LEU:O	2:F:168:THR:HA	2.05	0.56
1:B:373:LEU:HD13	1:B:384:ILE:CG2	2.35	0.56
1:D:320:ASN:O	1:D:324:THR:HG22	2.07	0.55
1:D:24:ASP:CB	1:D:28:ARG:NH2	2.58	0.55
1:B:239:ASP:HB3	1:B:243:LEU:HD12	1.88	0.55
2:E:54:LYS:HA	2:E:57:THR:HG22	1.88	0.55
1:D:120:SER:HB2	1:D:121:PRO:HD2	1.87	0.55
1:A:130:PRO:O	1:A:134:ARG:HG3	2.07	0.55
1:D:432:GLY:HA2	1:D:472:LYS:HE2	1.88	0.55
1:A:77:THR:HG23	1:A:86:VAL:CG1	2.37	0.55
1:A:313:LEU:HD13	1:A:321:VAL:CG2	2.36	0.55
2:E:158:LEU:HD21	2:F:100:TRP:CZ3	2.42	0.55
1:D:517:THR:HA	1:D:521:MET:HB2	1.89	0.55
1:A:74:GLY:HA3	1:A:111:SER:OG	2.06	0.55
2:G:107:MET:HB2	2:G:119:ARG:CZ	2.38	0.54
1:A:487:LEU:C	1:A:489:MET:H	2.11	0.54
1:B:456:TYR:HD2	1:B:459:ARG:NH2	2.04	0.54
2:F:27:ILE:HB	2:F:28:PRO:HD3	1.88	0.54
1:B:561:LYS:HB3	1:B:562:PRO:HD3	1.90	0.54
1:A:197:GLU:CD	1:A:197:GLU:H	2.10	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:53:LYS:HD3	2:F:54:LYS:H	1.73	0.54
1:A:349:ILE:O	1:A:352:LEU:HD23	2.07	0.54
1:B:237:GLN:HE21	1:B:275:GLY:HA3	1.73	0.54
2:F:168:THR:HG22	2:F:170:ARG:HG3	1.90	0.54
2:H:104:VAL:HG22	2:H:115:LEU:HD21	1.90	0.54
1:A:15:VAL:HG12	1:A:19:GLU:HB3	1.90	0.54
1:D:436:VAL:HG11	1:D:439:PHE:HD1	1.73	0.54
1:D:34:LYS:O	1:D:38:ILE:HG13	2.08	0.54
2:H:135:TRP:CD1	2:H:135:TRP:O	2.61	0.54
1:A:418:ARG:HH11	1:C:21:ARG:HH21	1.55	0.54
1:C:568:THR:HA	1:C:576:LYS:HB3	1.90	0.54
1:B:495:TYR:O	1:B:499:MET:HB2	2.08	0.54
1:C:468:LYS:C	1:C:470:VAL:H	2.10	0.54
2:E:6:ASN:ND2	2:E:9:GLU:H	2.06	0.54
1:B:436:VAL:HA	1:B:439:PHE:HB2	1.90	0.54
2:F:141:PHE:CE2	2:F:145:ARG:HD2	2.43	0.54
1:D:15:VAL:O	1:D:19:GLU:HG2	2.08	0.54
1:B:556:LEU:HA	1:B:560:VAL:HB	1.90	0.54
2:G:120:MET:O	2:G:124:ASN:HB2	2.08	0.53
1:C:561:LYS:HB3	1:C:562:PRO:HD3	1.88	0.53
1:C:156:PRO:HG3	1:C:195:VAL:HB	1.91	0.53
1:D:561:LYS:HA	1:D:564:LEU:HD12	1.89	0.53
1:B:179:PRO:CB	1:B:217:GLN:HE22	2.21	0.53
1:B:425:GLU:OE1	1:D:54:PHE:CZ	2.62	0.53
1:A:361:THR:HA	1:A:365:LEU:HB2	1.90	0.53
1:B:192:PHE:CZ	1:B:196:LEU:HD21	2.43	0.53
1:C:381:ARG:O	1:C:385:ILE:HG12	2.08	0.53
2:G:153:CYS:O	2:G:156:THR:HB	2.08	0.53
1:B:405:LEU:HD23	1:B:438:PHE:HE1	1.74	0.53
1:C:468:LYS:O	1:C:470:VAL:N	2.41	0.53
1:D:388:LEU:O	1:D:392:ASN:N	2.39	0.53
1:B:420:ARG:HE	1:B:458:ILE:HD13	1.73	0.53
1:D:113:ARG:HG2	1:D:153:VAL:HG11	1.90	0.53
1:B:183:ARG:NH2	1:B:217:GLN:NE2	2.56	0.53
1:C:470:VAL:O	1:C:470:VAL:HG12	2.08	0.53
1:C:317:CYS:HB2	1:C:320:ASN:HD21	1.74	0.53
2:G:53:LYS:HA	2:G:56:ASN:HD22	1.74	0.53
1:C:189:LEU:HD13	1:C:212:LEU:HD12	1.91	0.53
2:G:135:TRP:CZ2	2:G:163:ILE:HD12	2.44	0.53
1:A:236:PRO:C	1:A:238:GLU:H	2.13	0.53
1:D:436:VAL:HG11	1:D:439:PHE:CD1	2.44	0.53
1:D:170:PHE:CE2	1:D:174:CYS:SG	3.02	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:178:THR:HG22	1:C:181:VAL:H	1.72	0.52
1:D:454:HIS:HD2	2:F:128:TYR:CE1	2.21	0.52
1:B:134:ARG:NH2	1:B:134:ARG:HG3	2.23	0.52
1:A:381:ARG:HA	1:A:384:ILE:HG22	1.90	0.52
2:F:31:ARG:HG2	2:F:59:TYR:OH	2.09	0.52
1:A:313:LEU:HD13	1:A:321:VAL:HG21	1.91	0.52
1:B:467:LYS:HB2	1:B:507:VAL:CG1	2.39	0.52
2:E:6:ASN:HD21	2:E:9:GLU:H	1.57	0.52
1:A:409:VAL:HA	1:A:446:LEU:HD11	1.91	0.52
2:H:109:THR:OG1	2:H:111:CYS:HB3	2.09	0.52
2:F:164:ILE:C	2:F:166:GLN:H	2.11	0.52
1:B:427:MET:HA	1:B:427:MET:CE	2.40	0.52
2:F:56:ASN:O	2:F:60:LYS:HD3	2.09	0.52
1:A:180:MET:HE1	2:E:147:TRP:HE3	1.73	0.52
1:B:271:GLN:HE22	1:B:309:PHE:HA	1.73	0.52
1:C:13:ILE:HG12	1:C:14:ALA:N	2.21	0.52
1:B:319:GLU:O	1:B:323:MET:HB2	2.09	0.52
1:A:98:THR:CG2	1:A:140:TRP:CE3	2.92	0.52
1:C:424:ILE:HD12	1:C:458:ILE:CG1	2.39	0.52
1:B:274:VAL:HG23	1:B:275:GLY:N	2.25	0.52
2:G:145:ARG:HH21	2:G:152:LEU:N	2.07	0.52
2:E:15:ASP:CG	2:E:21:ARG:HH21	2.12	0.52
1:B:49:SER:O	1:B:53:PRO:HG2	2.09	0.52
1:A:94:GLU:OE1	1:A:131:LEU:HG	2.10	0.52
1:B:338:ASN:ND2	1:B:341:VAL:H	2.08	0.52
1:C:16:LEU:O	1:C:20:LEU:HB2	2.09	0.52
2:G:135:TRP:HZ2	2:G:163:ILE:HD12	1.75	0.52
1:B:268:THR:HG23	1:B:305:LYS:HD2	1.92	0.52
1:B:292:LYS:NZ	1:B:332:GLU:OE2	2.43	0.51
2:F:54:LYS:HA	2:F:57:THR:HG22	1.92	0.51
1:D:218:ASP:OD1	1:D:219:SER:N	2.44	0.51
2:H:105:LYS:O	2:H:106:LYS:HB3	2.10	0.51
1:B:36:SER:O	1:B:40:LEU:HD12	2.11	0.51
1:B:506:ASN:N	1:B:506:ASN:HD22	2.08	0.51
1:A:466:LEU:HB3	1:A:508:LEU:HD21	1.93	0.51
1:B:248:LEU:HD23	1:B:248:LEU:O	2.10	0.51
1:D:351:GLY:HA2	1:D:390:CYS:SG	2.50	0.51
1:A:167:ARG:CZ	1:A:200:ASN:HD22	2.23	0.51
1:C:201:VAL:O	1:C:206:ILE:HG12	2.10	0.51
1:A:427:MET:N	1:A:428:PRO:HD2	2.26	0.51
1:B:401:SER:O	1:B:404:LEU:HB3	2.10	0.51
2:E:97:CYS:HB3	2:F:100:TRP:CD1	2.46	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:369:PHE:HE1	1:B:384:ILE:HG23	1.75	0.51
1:A:178:THR:HG23	2:E:2:ASP:HB2	1.91	0.51
1:A:333:LEU:HB2	1:A:345:LEU:HD11	1.93	0.51
2:E:73:ASP:OD2	2:E:129:ARG:HD2	2.11	0.51
1:C:452:VAL:HG21	1:C:497:HIS:CE1	2.46	0.51
2:G:95:ILE:O	2:G:114:LEU:HB2	2.11	0.51
1:A:105:ARG:NH1	1:A:142:THR:HG22	2.26	0.51
1:D:368:LEU:O	1:D:371:ALA:N	2.44	0.51
1:A:179:PRO:O	1:A:183:ARG:HG3	2.11	0.51
2:G:160:TRP:O	2:G:163:ILE:HG22	2.11	0.51
2:F:1:MET:HE1	2:F:4:VAL:HG21	1.92	0.50
2:F:2:ASP:OD2	2:F:3:LYS:HD2	2.11	0.50
1:B:552:ASP:HB2	1:B:555:THR:OG1	2.10	0.50
1:D:271:GLN:HA	1:D:274:VAL:HG12	1.92	0.50
1:C:51:LEU:HA	1:C:54:PHE:HB3	1.92	0.50
1:A:131:LEU:HD23	1:A:131:LEU:C	2.32	0.50
2:H:100:TRP:CB	2:H:101:PRO:HD3	2.40	0.50
1:D:25:VAL:HB	1:D:27:LEU:HD23	1.93	0.50
2:E:77:PHE:O	2:E:78:TRP:HB2	2.11	0.50
1:B:96:LEU:O	1:B:98:THR:N	2.45	0.50
1:C:411:LEU:HD13	1:C:423:ILE:HD11	1.91	0.50
1:B:381:ARG:NH2	1:B:407:ALA:HA	2.26	0.50
1:C:553:ASN:O	1:C:557:GLN:HG2	2.11	0.50
1:A:205:ILE:HA	1:A:208:MET:HE3	1.94	0.50
1:D:77:THR:HG23	1:D:86:VAL:CG1	2.42	0.50
1:A:279:THR:HA	1:A:283:LEU:HB2	1.94	0.50
1:A:471:GLU:HG3	1:A:511:VAL:HG21	1.94	0.49
1:C:32:ILE:HD13	1:C:35:LEU:HD12	1.93	0.49
1:A:373:LEU:HD23	1:A:403:SER:CB	2.43	0.49
1:C:136:ALA:O	1:C:144:ARG:HG2	2.13	0.49
2:E:97:CYS:CB	2:F:100:TRP:CD1	2.95	0.49
1:C:216:GLU:HG2	2:G:7:ARG:NH1	2.27	0.49
1:B:178:THR:HG22	2:F:2:ASP:HB3	1.94	0.49
1:C:467:LYS:HE2	1:C:507:VAL:HG21	1.94	0.49
1:D:258:ARG:NH2	2:H:149:GLY:O	2.45	0.49
1:B:268:THR:HG21	1:B:308:GLU:HB3	1.93	0.49
1:D:410:GLU:HA	1:D:413:GLU:HG2	1.94	0.49
1:B:72:GLN:CG	1:B:76:PHE:HE2	2.24	0.49
1:A:381:ARG:O	1:A:384:ILE:HG22	2.13	0.49
2:F:62:MET:O	2:F:64:ASP:N	2.45	0.49
2:E:104:VAL:HG11	2:E:152:LEU:CD2	2.40	0.49
1:A:24:ASP:OD2	1:A:62:GLU:HG2	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:236:PRO:O	1:A:238:GLU:N	2.43	0.49
1:C:183:ARG:NH1	1:C:219:SER:OG	2.46	0.49
1:A:245:MET:O	1:A:249:ARG:HB2	2.12	0.49
1:C:498:ARG:O	1:C:501:THR:HB	2.12	0.49
2:E:114:LEU:HD12	2:E:114:LEU:H	1.78	0.49
1:B:130:PRO:O	1:B:134:ARG:HB2	2.13	0.49
1:B:350:MET:HG3	1:B:391:VAL:HG21	1.94	0.49
1:D:268:THR:HA	1:D:271:GLN:HG2	1.95	0.49
1:D:206:ILE:HG13	1:D:243:LEU:HD23	1.93	0.49
1:B:140:TRP:CD1	2:F:131:ASP:HB3	2.45	0.49
2:E:157:LEU:HD21	2:F:100:TRP:HE1	1.77	0.49
1:C:568:THR:HA	1:C:576:LYS:CB	2.42	0.49
1:B:189:LEU:HD21	1:B:205:ILE:HG23	1.94	0.49
2:H:160:TRP:CZ2	2:H:164:ILE:HD12	2.48	0.49
1:B:537:ARG:O	1:B:540:VAL:HB	2.13	0.49
2:E:87:SER:O	2:E:88:LEU:HD22	2.13	0.49
2:F:107:MET:HG2	2:F:107:MET:O	2.12	0.49
1:D:241:GLU:OE1	1:D:249:ARG:NH2	2.45	0.49
2:E:157:LEU:CD2	2:F:100:TRP:HE1	2.26	0.48
1:A:178:THR:CG2	2:E:2:ASP:HB3	2.43	0.48
2:E:97:CYS:HB3	2:F:100:TRP:HD1	1.77	0.48
1:B:369:PHE:CE1	1:B:384:ILE:HG23	2.48	0.48
1:A:317:CYS:O	1:A:321:VAL:HG22	2.13	0.48
2:F:136:VAL:HG22	2:F:136:VAL:O	2.12	0.48
1:C:331:LYS:HG2	1:C:368:LEU:HD21	1.95	0.48
2:H:59:TYR:O	2:H:62:MET:HG3	2.13	0.48
1:B:284:VAL:O	1:B:288:GLN:HG3	2.13	0.48
1:C:314:SER:C	1:C:316:ASP:N	2.64	0.48
1:C:456:TYR:HD2	1:C:459:ARG:NH2	2.12	0.48
2:G:12:GLN:O	2:G:16:LEU:HG	2.13	0.48
1:C:405:LEU:CD1	1:C:443:LEU:HD13	2.43	0.48
1:C:111:SER:O	1:C:115:ILE:HG12	2.13	0.48
1:C:29:LEU:HD11	1:C:64:GLU:HG2	1.95	0.48
1:D:202:LYS:HA	1:D:206:ILE:HG12	1.95	0.48
2:E:145:ARG:HG2	2:E:150:LEU:O	2.13	0.48
2:F:100:TRP:HB2	2:F:101:PRO:CD	2.42	0.48
1:C:113:ARG:NH1	1:C:153:VAL:HG13	2.29	0.48
1:D:375:ASP:OD2	1:D:376:GLU:N	2.47	0.48
1:A:316:ASP:OD2	1:A:317:CYS:N	2.47	0.48
2:F:164:ILE:C	2:F:166:GLN:N	2.67	0.48
1:B:26:GLN:HE21	1:B:30:ASN:HD21	1.61	0.48
1:D:460:GLU:OE1	2:F:130:LYS:NZ	2.47	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:9:GLU:CD	2:H:9:GLU:H	2.17	0.48
2:F:59:TYR:O	2:F:63:GLU:HB2	2.13	0.48
1:A:420:ARG:HA	1:A:423:ILE:HD11	1.95	0.48
2:E:70:HIS:ND1	2:E:170:ARG:HD3	2.29	0.48
1:B:424:ILE:HG12	1:B:450:TRP:CE3	2.49	0.48
1:A:464:SER:O	1:A:468:LYS:HD3	2.14	0.48
1:D:28:ARG:NH1	1:D:61:ASP:OD1	2.47	0.47
2:G:100:TRP:HB3	2:G:101:PRO:CD	2.40	0.47
1:D:56:THR:C	1:D:58:THR:H	2.18	0.47
1:B:197:GLU:CD	1:B:197:GLU:H	2.18	0.47
2:F:70:HIS:CG	2:F:170:ARG:HD2	2.49	0.47
1:B:412:ALA:HB1	1:B:450:TRP:HZ2	1.79	0.47
2:H:95:ILE:HG22	2:H:114:LEU:H	1.78	0.47
2:E:123:GLU:HA	2:E:126:LYS:HG2	1.95	0.47
1:C:37:THR:O	1:C:41:ALA:N	2.34	0.47
1:C:255:LYS:HE2	1:C:255:LYS:N	2.21	0.47
1:A:405:LEU:HB3	1:A:406:PRO:HD3	1.96	0.47
1:D:264:ALA:HB2	1:D:290:LEU:HG	1.96	0.47
1:B:205:ILE:CG2	1:B:231:ILE:HD11	2.44	0.47
1:C:81:GLY:HA3	1:C:85:TYR:HD1	1.80	0.47
1:A:455:VAL:HG13	2:G:127:LEU:HD22	1.96	0.47
1:A:183:ARG:HD3	1:A:219:SER:OG	2.15	0.47
1:B:548:GLY:HA3	1:B:586:LEU:HD21	1.97	0.47
1:B:381:ARG:HG3	1:B:411:LEU:HD21	1.96	0.47
1:A:207:PRO:O	1:A:211:ASN:ND2	2.47	0.47
1:C:279:THR:O	1:C:283:LEU:HB2	2.15	0.47
2:H:1:MET:H2	2:H:136:VAL:HG22	1.78	0.47
1:C:428:PRO:HD3	1:C:465:ASN:ND2	2.30	0.47
1:D:432:GLY:CA	1:D:472:LYS:HE2	2.44	0.47
1:A:516:ILE:HG23	1:A:520:HIS:HD2	1.80	0.47
2:F:135:TRP:CH2	2:F:163:ILE:HD12	2.50	0.47
1:B:30:ASN:O	1:B:33:LYS:HG3	2.15	0.47
1:A:176:ASP:OD1	1:A:178:THR:OG1	2.32	0.47
1:C:440:ASP:C	1:C:442:LYS:H	2.17	0.47
1:C:536:VAL:O	1:C:540:VAL:HG23	2.15	0.47
1:A:422:ALA:HB2	1:C:21:ARG:CD	2.38	0.47
2:H:112:ILE:O	2:H:112:ILE:CG2	2.56	0.47
1:D:350:MET:HG3	1:D:391:VAL:HG22	1.96	0.47
1:C:547:ILE:HD12	1:C:551:LEU:HD11	1.97	0.47
1:C:67:LEU:CD2	1:C:107:LYS:HG3	2.45	0.47
2:F:21:ARG:O	2:F:22:SER:HB3	2.14	0.46
2:F:163:ILE:O	2:F:163:ILE:CD1	2.62	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:325:GLN:HA	1:B:325:GLN:NE2	2.30	0.46
1:B:144:ARG:HG3	1:B:144:ARG:NH1	2.30	0.46
1:B:174:CYS:SG	1:B:208:MET:HG2	2.55	0.46
1:B:87:HIS:HA	1:B:90:LEU:HD13	1.97	0.46
2:H:136:VAL:HG12	2:H:139:TYR:CZ	2.51	0.46
2:E:168:THR:HG23	2:E:170:ARG:NE	2.28	0.46
2:G:1:MET:HG2	2:G:136:VAL:HG21	1.98	0.46
1:D:271:GLN:C	1:D:273:ALA:H	2.18	0.46
1:C:32:ILE:O	1:C:35:LEU:HB2	2.15	0.46
1:A:201:VAL:O	1:A:206:ILE:HG12	2.14	0.46
2:F:100:TRP:CB	2:F:101:PRO:HD3	2.44	0.46
1:D:94:GLU:OE1	1:D:131:LEU:HD22	2.16	0.46
2:E:144:PHE:CE1	2:E:160:TRP:HB2	2.51	0.46
1:D:436:VAL:HG22	1:D:438:PHE:HB3	1.98	0.46
1:C:90:LEU:HB2	1:C:91:PRO:HD3	1.96	0.46
1:C:105:ARG:O	1:C:108:ALA:HB3	2.15	0.46
2:E:104:VAL:CG1	2:E:152:LEU:HD21	2.44	0.46
1:A:502:LEU:CD1	1:A:528:MET:SD	3.04	0.46
1:A:498:ARG:O	1:A:501:THR:HB	2.15	0.46
1:C:258:ARG:NH2	2:G:149:GLY:O	2.49	0.46
1:C:455:VAL:HB	1:C:458:ILE:HG22	1.97	0.46
1:C:183:ARG:HD3	1:C:219:SER:HB2	1.97	0.46
1:B:37:THR:HA	1:B:40:LEU:HB2	1.98	0.46
2:E:42:HIS:CB	2:E:43:PRO:CD	2.93	0.46
2:G:123:GLU:HA	2:G:126:LYS:HG2	1.97	0.46
1:C:405:LEU:HD12	1:C:443:LEU:HD13	1.97	0.46
1:D:318:ARG:O	1:D:322:ILE:HG13	2.15	0.46
1:C:322:ILE:HG21	1:C:356:LEU:HD21	1.97	0.46
1:B:497:HIS:O	1:B:500:THR:OG1	2.28	0.46
1:B:340:HIS:CD2	1:B:340:HIS:N	2.83	0.46
2:F:114:LEU:HD23	2:F:117:LEU:HD23	1.98	0.46
1:B:159:SER:OG	1:B:162:VAL:HG23	2.16	0.46
1:B:98:THR:HG22	1:B:140:TRP:HE3	1.81	0.46
1:A:418:ARG:CZ	1:A:418:ARG:HB2	2.44	0.46
1:A:96:LEU:C	1:A:98:THR:H	2.19	0.46
1:C:268:THR:HG23	1:C:305:LYS:HG2	1.97	0.46
1:C:456:TYR:CZ	1:C:460:GLU:HG3	2.51	0.46
1:B:128:PHE:O	1:B:131:LEU:HB3	2.16	0.46
1:B:201:VAL:O	1:B:206:ILE:HG12	2.16	0.46
1:A:24:ASP:OD1	1:A:61:ASP:HB3	2.16	0.46
1:B:171:ARG:NH2	1:B:171:ARG:HB2	2.25	0.46
1:C:338:ASN:HD21	1:C:340:HIS:HB2	1.80	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:61:ASP:CG	1:C:62:GLU:H	2.19	0.46
2:E:6:ASN:HD22	2:E:6:ASN:H	1.65	0.45
2:H:144:PHE:CD1	2:H:160:TRP:HB2	2.52	0.45
1:A:222:LEU:C	1:A:222:LEU:HD23	2.37	0.45
1:C:479:HIS:HA	1:C:483:ILE:HB	1.98	0.45
1:A:52:LEU:HD13	1:A:52:LEU:HA	1.86	0.45
2:F:113:CYS:O	2:F:117:LEU:HD22	2.15	0.45
2:F:2:ASP:OD1	2:F:134:VAL:HG21	2.16	0.45
2:F:98:LYS:O	2:F:99:GLN:HB3	2.16	0.45
1:C:15:VAL:O	1:C:19:GLU:HG2	2.17	0.45
1:C:286:ALA:HA	1:C:289:ASN:HD22	1.81	0.45
1:D:194:LYS:HD3	1:D:234:LEU:HD21	1.99	0.45
2:F:31:ARG:HH22	2:F:35:LEU:CD1	2.30	0.45
1:D:22:ASN:CB	1:D:23:GLU:O	2.56	0.45
2:E:107:MET:HG3	2:E:119:ARG:NH1	2.31	0.45
1:B:561:LYS:HA	1:B:564:LEU:HD12	1.97	0.45
2:G:168:THR:C	2:G:170:ARG:H	2.20	0.45
1:A:271:GLN:HE22	1:A:309:PHE:HA	1.81	0.45
2:H:40:GLU:O	2:H:41:PHE:CB	2.64	0.45
1:B:545:GLN:HE21	1:B:585:VAL:HG11	1.82	0.45
1:B:556:LEU:HD22	1:B:588:LEU:HD11	1.98	0.45
2:H:108:SER:O	2:H:109:THR:HB	2.17	0.45
1:B:580:GLN:HA	1:B:583:LEU:HD12	1.99	0.45
1:B:406:PRO:O	1:B:410:GLU:HB2	2.17	0.45
1:C:258:ARG:NH1	2:G:149:GLY:O	2.50	0.45
2:F:99:GLN:HG2	2:F:102:GLU:HB2	1.99	0.45
1:A:537:ARG:O	1:A:540:VAL:HB	2.17	0.45
1:B:96:LEU:C	1:B:98:THR:H	2.20	0.45
1:A:350:MET:HB3	1:A:391:VAL:CG2	2.45	0.45
1:A:524:THR:HG23	1:A:527:ARG:NH2	2.32	0.45
1:D:456:TYR:CZ	2:F:130:LYS:HD2	2.52	0.45
1:B:59:ILE:CG2	1:B:66:LEU:CD2	2.94	0.45
2:E:100:TRP:CZ3	2:E:104:VAL:HG21	2.52	0.45
1:C:456:TYR:CG	2:E:128:TYR:HB3	2.52	0.45
1:A:417:TRP:HZ3	1:A:421:LEU:HD12	1.81	0.45
1:A:502:LEU:HD11	1:A:528:MET:SD	2.57	0.45
1:A:138:GLY:O	1:A:144:ARG:NH1	2.50	0.45
2:G:98:LYS:O	2:G:99:GLN:HB3	2.17	0.45
2:F:111:CYS:HB3	2:F:113:CYS:HB3	1.98	0.45
1:D:25:VAL:HG12	1:D:26:GLN:H	1.81	0.45
1:C:479:HIS:HB2	1:C:483:ILE:HD12	1.97	0.45
1:B:318:ARG:O	1:B:322:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:452:VAL:HG23	1:A:497:HIS:NE2	2.31	0.45
1:B:363:GLU:HG2	1:B:364:HIS:CD2	2.51	0.45
2:G:135:TRP:CD1	2:G:136:VAL:HG23	2.51	0.45
1:C:544:LEU:HD23	1:C:547:ILE:HD11	1.99	0.45
2:H:138:CYS:SG	2:H:140:CYS:HB3	2.57	0.45
1:B:39:ALA:HB3	1:B:79:LEU:HD23	1.99	0.45
1:B:24:ASP:HB3	1:B:25:VAL:H	1.53	0.44
1:C:448:MET:CG	1:C:451:LEU:HD12	2.47	0.44
1:B:46:ARG:O	1:B:50:GLU:N	2.44	0.44
1:B:90:LEU:N	1:B:91:PRO:CD	2.80	0.44
1:D:505:ILE:HD13	1:D:525:VAL:HG22	2.00	0.44
1:A:319:GLU:O	1:A:323:MET:HB2	2.17	0.44
1:C:466:LEU:HD12	1:C:469:LEU:HD23	2.00	0.44
1:A:200:ASN:OD1	1:A:200:ASN:N	2.50	0.44
1:C:29:LEU:HD13	1:C:65:VAL:HA	2.00	0.44
1:C:22:ASN:O	1:C:23:GLU:HB3	2.18	0.44
1:D:90:LEU:O	1:D:91:PRO:C	2.54	0.44
1:A:67:LEU:HD11	1:A:103:VAL:HG12	2.00	0.44
2:E:97:CYS:CB	2:F:100:TRP:HD1	2.30	0.44
2:E:11:LEU:HD22	2:E:21:ARG:HD3	1.99	0.44
1:A:215:ASP:O	1:A:216:GLU:C	2.55	0.44
1:A:417:TRP:CZ3	1:A:421:LEU:HD12	2.52	0.44
1:A:528:MET:C	1:A:530:GLY:H	2.21	0.44
1:D:288:GLN:NE2	1:D:325:GLN:HB3	2.32	0.44
2:E:1:MET:SD	2:E:25:GLY:HA2	2.58	0.44
1:A:487:LEU:HD22	1:A:524:THR:HG21	2.00	0.44
1:B:90:LEU:HD23	1:B:131:LEU:HD13	1.99	0.44
1:A:424:ILE:HG12	1:A:450:TRP:CE3	2.52	0.44
1:A:28:ARG:O	1:A:32:ILE:HG13	2.18	0.44
1:D:168:GLN:NE2	1:D:171:ARG:HE	2.15	0.44
1:B:77:THR:HG21	1:B:118:GLU:OE1	2.17	0.44
1:B:412:ALA:HB1	1:B:450:TRP:CZ2	2.51	0.44
1:C:497:HIS:CD2	1:C:497:HIS:N	2.86	0.44
1:B:545:GLN:NE2	1:B:585:VAL:HG11	2.33	0.44
1:A:506:ASN:HD21	1:A:543:SER:HA	1.83	0.44
1:A:360:ASN:HA	1:A:363:GLU:HB2	1.99	0.44
2:F:118:LEU:HB3	2:F:140:CYS:HA	2.00	0.44
1:D:495:TYR:HB3	1:D:533:VAL:HG21	2.00	0.44
1:B:402:GLN:O	1:B:403:SER:CB	2.66	0.44
1:B:100:GLU:HG2	2:F:132:PRO:HB3	2.00	0.44
2:F:145:ARG:CZ	2:F:152:LEU:HD22	2.47	0.44
1:D:202:LYS:HA	1:D:206:ILE:CG1	2.47	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:171:ARG:HB2	1:A:171:ARG:HE	1.56	0.44
1:B:424:ILE:HD11	1:B:458:ILE:HG23	1.98	0.44
1:B:542:LYS:HE2	1:B:578:PHE:CE1	2.53	0.44
1:D:540:VAL:O	1:D:543:SER:HB3	2.18	0.44
2:G:13:LEU:HB2	2:G:58:LEU:HD13	1.99	0.44
1:D:155:TYR:CZ	1:D:163:LYS:HD3	2.52	0.44
2:G:138:CYS:HB3	2:G:143:CYS:SG	2.58	0.44
1:D:54:PHE:CD2	1:D:54:PHE:C	2.91	0.44
2:E:154:GLU:HG3	2:F:100:TRP:CH2	2.53	0.44
2:H:54:LYS:HD2	2:H:57:THR:HG21	1.99	0.44
1:C:448:MET:HG2	1:C:451:LEU:HD12	1.99	0.44
1:B:173:LEU:O	1:B:176:ASP:HB2	2.18	0.44
1:D:291:MET:HE3	1:D:333:LEU:HD12	2.00	0.44
1:A:373:LEU:HD23	1:A:403:SER:HB2	2.00	0.43
1:A:508:LEU:O	1:A:512:CYS:SG	2.75	0.43
1:B:25:VAL:HB	1:B:26:GLN:H	1.60	0.43
1:B:72:GLN:HG3	1:B:76:PHE:CE2	2.50	0.43
1:D:224:ALA:O	1:D:227:ALA:N	2.51	0.43
1:C:127:HIS:C	1:C:130:PRO:HD2	2.38	0.43
2:E:138:CYS:HB3	2:E:143:CYS:SG	2.58	0.43
1:D:179:PRO:O	1:D:180:MET:C	2.57	0.43
1:D:61:ASP:OD1	1:D:62:GLU:N	2.46	0.43
1:B:321:VAL:O	1:B:325:GLN:HB2	2.17	0.43
2:G:113:CYS:HB3	2:G:116:CYS:H	1.83	0.43
1:B:417:TRP:HB3	1:B:420:ARG:HH11	1.83	0.43
2:F:64:ASP:HA	2:F:67:LYS:HB3	1.99	0.43
1:D:547:ILE:HG13	1:D:547:ILE:H	1.65	0.43
1:C:571:GLN:O	1:C:571:GLN:HG2	2.19	0.43
2:G:108:SER:H	2:G:119:ARG:NH1	2.16	0.43
1:C:29:LEU:O	1:C:31:SER:N	2.52	0.43
1:A:159:SER:O	1:A:163:LYS:HG3	2.17	0.43
1:C:52:LEU:HD23	1:C:52:LEU:HA	1.66	0.43
2:H:125:ARG:NE	2:H:133:LEU:HD11	2.33	0.43
1:C:374:LYS:HA	1:C:381:ARG:HH21	1.83	0.43
1:A:189:LEU:HD11	1:A:205:ILE:HG23	2.01	0.43
1:D:412:ALA:HB2	1:D:423:ILE:HG21	2.01	0.43
1:C:397:ILE:HD11	1:C:434:LEU:HA	2.00	0.43
1:D:262:MET:O	1:D:266:LYS:HG2	2.18	0.43
1:B:179:PRO:O	1:B:183:ARG:HG3	2.18	0.43
1:B:316:ASP:HB3	1:B:317:CYS:H	1.61	0.43
1:A:412:ALA:CB	1:A:450:TRP:HZ2	2.32	0.43
1:D:317:CYS:O	1:D:321:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:141:PHE:O	1:D:145:THR:HG23	2.18	0.43
1:C:222:LEU:C	1:C:222:LEU:HD12	2.39	0.43
2:F:31:ARG:CB	2:F:31:ARG:HH11	2.17	0.43
2:F:100:TRP:O	2:F:104:VAL:CG2	2.61	0.43
2:E:95:ILE:HD12	2:H:110:ASN:HB3	2.00	0.43
1:C:197:GLU:CG	1:C:200:ASN:HD22	2.29	0.43
1:D:95:SER:O	1:D:98:THR:HB	2.19	0.43
1:D:452:VAL:O	1:D:452:VAL:HG22	2.19	0.43
1:A:256:SER:OG	1:A:259:VAL:HG23	2.18	0.43
2:E:97:CYS:HB2	2:F:100:TRP:CD1	2.54	0.43
1:B:89:LEU:O	1:B:92:PRO:HD2	2.18	0.43
1:A:155:TYR:CZ	1:A:163:LYS:HB3	2.54	0.43
1:D:254:ASP:OD2	1:D:255:LYS:N	2.52	0.43
1:D:352:LEU:HA	1:D:355:ILE:HD12	2.00	0.43
2:F:145:ARG:O	2:F:148:PHE:O	2.36	0.43
1:D:25:VAL:HB	1:D:27:LEU:CD2	2.48	0.43
1:B:145:THR:HG22	1:B:181:VAL:HA	2.00	0.43
1:C:226:GLU:HB2	1:C:262:MET:CE	2.49	0.43
1:B:456:TYR:CZ	2:H:130:LYS:HB2	2.54	0.43
1:B:418:ARG:HG3	1:D:21:ARG:NH1	2.26	0.43
1:B:437:GLU:HG2	1:B:438:PHE:N	2.31	0.42
1:C:21:ARG:HA	1:C:21:ARG:HE	1.83	0.42
1:B:216:GLU:CG	2:F:22:SER:HB3	2.49	0.42
2:H:169:TYR:CD1	2:H:172:LEU:HA	2.47	0.42
1:B:501:THR:O	1:B:505:ILE:HG13	2.19	0.42
1:B:288:GLN:NE2	1:B:325:GLN:HE21	2.17	0.42
1:C:428:PRO:HD3	1:C:465:ASN:HD22	1.83	0.42
2:H:4:VAL:HG12	2:H:65:GLY:HA3	2.01	0.42
1:C:453:ASP:O	1:C:459:ARG:HD3	2.19	0.42
1:C:67:LEU:HD23	1:C:107:LYS:HG3	2.01	0.42
1:C:369:PHE:CZ	1:C:373:LEU:HD22	2.54	0.42
1:D:72:GLN:O	1:D:76:PHE:HD1	2.02	0.42
1:B:402:GLN:HA	1:B:405:LEU:HD21	2.00	0.42
1:C:463:THR:O	1:C:467:LYS:N	2.40	0.42
1:D:358:LYS:HG3	1:D:394:VAL:HG13	2.00	0.42
1:B:58:THR:HG21	1:D:425:GLU:OE2	2.19	0.42
1:D:183:ARG:NH2	2:H:149:GLY:HA2	2.32	0.42
2:F:152:LEU:HD12	2:F:152:LEU:O	2.19	0.42
1:C:179:PRO:O	1:C:183:ARG:HG3	2.19	0.42
1:C:94:GLU:OE1	1:C:131:LEU:HD13	2.19	0.42
1:C:98:THR:HG23	1:C:140:TRP:HD1	1.84	0.42
1:C:96:LEU:HA	1:C:99:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:413:GLU:HG2	1:A:413:GLU:O	2.19	0.42
1:A:29:LEU:HD12	1:A:29:LEU:HA	1.75	0.42
1:D:447:CYS:HA	1:D:450:TRP:CE3	2.54	0.42
2:H:1:MET:HB3	2:H:2:ASP:H	1.46	0.42
1:C:427:MET:N	1:C:428:PRO:CD	2.79	0.42
1:B:338:ASN:HD21	1:B:340:HIS:HB2	1.84	0.42
1:C:16:LEU:HD12	1:C:54:PHE:CE1	2.53	0.42
1:A:353:SER:N	1:A:354:PRO:HD2	2.35	0.42
1:C:280:LYS:HB2	1:C:280:LYS:HE3	1.86	0.42
1:C:338:ASN:ND2	1:C:341:VAL:HG23	2.30	0.42
2:E:102:GLU:O	2:E:107:MET:HA	2.20	0.42
1:D:381:ARG:O	1:D:385:ILE:HG12	2.19	0.42
2:E:19:LEU:O	2:E:20:GLU:C	2.58	0.42
1:B:452:VAL:O	1:B:452:VAL:HG22	2.19	0.42
2:G:99:GLN:HA	2:H:98:LYS:O	2.19	0.42
1:C:556:LEU:HA	1:C:560:VAL:HB	2.01	0.42
1:A:412:ALA:HB1	1:A:450:TRP:CZ2	2.54	0.42
1:A:547:ILE:HA	1:A:550:ILE:HD12	2.02	0.42
1:C:133:LYS:HE2	1:C:169:TYR:CE2	2.55	0.42
1:A:115:ILE:O	1:A:119:HIS:HD2	2.02	0.42
1:B:140:TRP:CG	2:F:132:PRO:HD2	2.55	0.42
1:B:216:GLU:CB	2:F:22:SER:HB3	2.48	0.42
1:C:333:LEU:HB2	1:C:345:LEU:HD22	2.02	0.42
1:C:216:GLU:HG3	2:G:11:LEU:HD21	2.01	0.42
1:C:29:LEU:O	1:C:32:ILE:N	2.52	0.42
2:E:88:LEU:HB3	2:E:89:ASN:H	1.59	0.42
2:F:98:LYS:O	2:F:99:GLN:CB	2.67	0.42
1:C:473:PHE:O	1:C:474:GLY:O	2.37	0.42
1:D:258:ARG:NH1	2:H:149:GLY:O	2.52	0.42
1:A:196:LEU:HD13	1:A:200:ASN:HB2	2.02	0.42
1:D:352:LEU:HD23	1:D:355:ILE:HD12	2.01	0.42
1:C:188:LYS:HD2	1:C:191:GLU:OE2	2.19	0.42
1:B:297:GLU:N	1:B:297:GLU:OE2	2.50	0.42
2:G:106:LYS:HB2	2:G:107:MET:CE	2.49	0.42
1:A:425:GLU:OE1	1:C:17:ILE:HD13	2.20	0.42
1:A:576:LYS:O	1:A:580:GLN:HB2	2.20	0.42
1:B:44:VAL:HG13	1:B:45:GLU:HG3	2.01	0.42
1:C:572:ASP:O	1:C:576:LYS:HG2	2.20	0.41
1:D:436:VAL:HG21	1:D:439:PHE:CD1	2.55	0.41
1:D:456:TYR:HA	1:D:459:ARG:HE	1.83	0.41
1:D:216:GLU:HB3	2:H:21:ARG:O	2.20	0.41
1:B:431:ALA:HB1	1:B:473:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:266:LYS:O	1:C:270:LEU:HG	2.19	0.41
1:D:222:LEU:C	1:D:222:LEU:HD23	2.40	0.41
1:B:22:ASN:C	1:B:24:ASP:N	2.69	0.41
1:B:72:GLN:HE21	1:B:72:GLN:HB2	1.60	0.41
1:D:26:GLN:OE1	1:D:26:GLN:HA	2.19	0.41
1:A:279:THR:O	1:A:284:VAL:HG23	2.20	0.41
1:B:91:PRO:HB2	1:B:92:PRO:HD3	2.02	0.41
1:D:35:LEU:HA	1:D:38:ILE:HD12	2.02	0.41
2:G:113:CYS:O	2:G:117:LEU:HD13	2.19	0.41
2:F:111:CYS:CB	2:F:113:CYS:H	2.33	0.41
1:D:561:LYS:N	1:D:562:PRO:CD	2.84	0.41
1:C:96:LEU:C	1:C:98:THR:H	2.24	0.41
1:B:522:LEU:HB3	1:B:523:PRO:HD3	2.01	0.41
2:H:94:ALA:O	2:H:95:ILE:HG13	2.21	0.41
1:A:128:PHE:O	1:A:131:LEU:HB3	2.20	0.41
1:C:456:TYR:OH	1:C:460:GLU:HG3	2.21	0.41
1:A:417:TRP:CB	1:A:455:VAL:HG21	2.50	0.41
1:C:61:ASP:H	1:C:66:LEU:HD11	1.85	0.41
2:E:138:CYS:SG	2:E:139:TYR:N	2.93	0.41
2:H:13:LEU:O	2:H:17:LEU:HB2	2.21	0.41
2:H:122:HIS:CD2	2:H:122:HIS:C	2.93	0.41
2:E:36:LYS:HE2	2:E:36:LYS:HB3	1.90	0.41
2:H:94:ALA:C	2:H:95:ILE:HG13	2.41	0.41
1:D:221:ARG:HD2	1:D:254:ASP:OD1	2.21	0.41
1:D:29:LEU:C	1:D:29:LEU:HD13	2.40	0.41
1:B:245:MET:HB3	1:B:249:ARG:NH1	2.36	0.41
1:B:134:ARG:CG	1:B:134:ARG:NH2	2.82	0.41
1:C:287:PHE:CE2	1:C:291:MET:SD	3.14	0.41
1:A:446:LEU:C	1:A:448:MET:H	2.24	0.41
1:D:238:GLU:CD	1:D:238:GLU:H	2.23	0.41
1:C:396:GLY:H	1:C:399:GLN:NE2	2.18	0.41
1:A:417:TRP:HB3	1:A:455:VAL:HG21	2.03	0.41
1:D:29:LEU:HD23	1:D:65:VAL:HA	2.02	0.41
2:E:110:ASN:HD21	2:H:95:ILE:HG23	1.86	0.41
2:G:100:TRP:O	2:G:104:VAL:HG23	2.21	0.41
1:D:377:CYS:HA	1:D:378:PRO:HD3	1.81	0.41
1:D:452:VAL:CG2	1:D:496:LEU:HB3	2.47	0.41
1:C:178:THR:HA	1:C:179:PRO:HD3	1.98	0.41
1:A:381:ARG:NH2	1:A:407:ALA:HA	2.35	0.41
1:D:198:LEU:O	1:D:202:LYS:HD3	2.21	0.41
1:C:405:LEU:N	1:C:406:PRO:HD2	2.36	0.41
1:C:52:LEU:HB2	1:C:53:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:109:THR:O	2:E:111:CYS:N	2.54	0.41
2:H:55:MET:HG2	2:H:55:MET:O	2.21	0.41
1:A:278:ILE:HD12	1:A:278:ILE:H	1.86	0.41
2:G:144:PHE:CG	2:G:160:TRP:HD1	2.39	0.41
1:B:151:PHE:CD1	1:B:170:PHE:HD2	2.39	0.41
1:D:188:LYS:HD2	1:D:191:GLU:OE1	2.21	0.41
1:D:424:ILE:HG12	1:D:450:TRP:CE3	2.56	0.40
1:A:516:ILE:HG13	1:A:516:ILE:H	1.76	0.40
1:C:417:TRP:HA	1:C:420:ARG:NH1	2.36	0.40
1:B:344:ALA:O	1:B:347:SER:OG	2.30	0.40
1:B:240:LEU:HA	1:B:240:LEU:HD23	1.80	0.40
1:C:427:MET:HB3	1:C:465:ASN:HD21	1.86	0.40
2:E:1:MET:HA	2:E:4:VAL:HG23	2.02	0.40
2:G:31:ARG:HG2	2:G:59:TYR:OH	2.22	0.40
1:C:351:GLY:HA2	1:C:390:CYS:SG	2.61	0.40
1:C:21:ARG:HB3	1:C:22:ASN:H	1.66	0.40
2:E:100:TRP:CD1	2:F:95:ILE:HG22	2.57	0.40
2:F:109:THR:HG22	2:F:119:ARG:NH2	2.32	0.40
2:F:37:LYS:C	2:F:39:LYS:H	2.25	0.40
2:H:119:ARG:HG2	2:H:119:ARG:HH21	1.86	0.40
2:E:27:ILE:H	2:E:27:ILE:HG12	1.74	0.40
1:D:466:LEU:O	1:D:470:VAL:HG23	2.22	0.40
1:A:33:LYS:CD	1:A:33:LYS:N	2.83	0.40
1:D:556:LEU:HD23	1:D:560:VAL:HG21	2.04	0.40
1:B:86:VAL:HG13	1:B:119:HIS:CE1	2.55	0.40
2:G:99:GLN:HE21	2:G:102:GLU:HB2	1.86	0.40
1:D:119:HIS:O	1:D:157:ARG:NH1	2.55	0.40
1:A:42:LEU:O	1:A:46:ARG:HB2	2.22	0.40
1:A:50:GLU:C	1:A:53:PRO:HD2	2.42	0.40
1:A:563:ILE:HD13	1:A:563:ILE:HA	1.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	573/589 (97%)	505 (88%)	53 (9%)	15 (3%)	8	41
1	B	573/589 (97%)	507 (88%)	57 (10%)	9 (2%)	14	55
1	C	575/589 (98%)	502 (87%)	65 (11%)	8 (1%)	16	58
1	D	575/589 (98%)	477 (83%)	85 (15%)	13 (2%)	10	45
2	E	157/174 (90%)	127 (81%)	20 (13%)	10 (6%)	2	15
2	F	146/174 (84%)	112 (77%)	24 (16%)	10 (7%)	2	14
2	G	136/174 (78%)	114 (84%)	17 (12%)	5 (4%)	5	31
2	H	137/174 (79%)	106 (77%)	18 (13%)	13 (10%)	1	7
All	All	2872/3052 (94%)	2450 (85%)	339 (12%)	83 (3%)	7	38

All (83) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	ALA
1	B	97	ALA
1	B	316	ASP
1	B	317	CYS
1	B	401	SER
1	C	25	VAL
1	C	474	GLY
2	E	42	HIS
2	E	106	LYS
2	E	110	ASN
2	F	2	ASP
2	F	63	GLU
2	F	138	CYS
2	G	100	TRP
2	H	3	LYS
2	H	7	ARG
2	H	72	PRO
1	A	237	GLN
1	A	316	ASP
1	A	443	LEU
1	C	315	ALA
1	C	469	LEU
1	D	43	GLY
1	D	160	SER
1	D	369	PHE
1	D	386	SER
1	D	573	VAL

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Mol	Chain	Res	Type
2	E	92	VAL
2	E	105	LYS
2	E	136	VAL
2	E	152	LEU
2	E	169	TYR
2	F	52	MET
2	H	70	HIS
2	H	95	ILE
2	H	100	TRP
2	H	106	LYS
2	H	136	VAL
2	H	152	LEU
1	A	50	GLU
1	A	199	ASP
1	A	320	ASN
1	A	573	VAL
1	B	549	PRO
1	C	441	GLU
1	D	401	SER
1	D	522	LEU
1	D	571	GLN
2	F	5	LEU
2	H	24	TRP
1	A	48	ARG
1	A	349	ILE
1	A	488	ALA
1	B	25	VAL
1	D	564	LEU
2	F	22	SER
2	G	105	LYS
2	H	65	GLY
1	A	97	ALA
1	A	348	VAL
1	A	515	ASP
1	B	403	SER
1	C	44	VAL
1	C	471	GLU
1	C	515	ASP
1	D	57	ASP
1	D	306	VAL
2	F	93	ASP
2	H	21	ARG

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Mol	Chain	Res	Type
2	H	107	MET
1	B	209	PHE
1	B	210	SER
1	D	547	ILE
1	D	553	ASN
2	F	169	TYR
2	G	152	LEU
2	E	90	PRO
2	F	136	VAL
2	G	112	ILE
2	G	136	VAL
1	A	482	ILE
2	E	43	PRO
2	F	90	PRO

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	501/512 (98%)	455 (91%)	46 (9%)	13	45
1	B	501/512 (98%)	448 (89%)	53 (11%)	10	35
1	C	502/512 (98%)	448 (89%)	54 (11%)	9	34
1	D	503/512 (98%)	454 (90%)	49 (10%)	12	41
2	E	138/157 (88%)	116 (84%)	22 (16%)	4	13
2	F	134/157 (85%)	110 (82%)	24 (18%)	2	10
2	G	128/157 (82%)	95 (74%)	33 (26%)	1	2
2	H	128/157 (82%)	107 (84%)	21 (16%)	3	12
All	All	2535/2676 (95%)	2233 (88%)	302 (12%)	8	27

All (302) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	51	LEU
1	A	52	LEU

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Mol	Chain	Res	Type
1	A	60	TYR
1	A	67	LEU
1	A	72	GLN
1	A	78	THR
1	A	85	TYR
1	A	110	GLU
1	A	111	SER
1	A	125	GLU
1	A	139	ASP
1	A	152	SER
1	A	159	SER
1	A	175	SER
1	A	178	THR
1	A	187	SER
1	A	194	LYS
1	A	196	LEU
1	A	200	ASN
1	A	222	LEU
1	A	235	LEU
1	A	237	GLN
1	A	238	GLU
1	A	241	GLU
1	A	250	GLN
1	A	270	LEU
1	A	274	VAL
1	A	283	LEU
1	A	327	LEU
1	A	348	VAL
1	A	355	ILE
1	A	359	ASP
1	A	365	LEU
1	A	368	LEU
1	A	370	LEU
1	A	399	GLN
1	A	408	ILE
1	A	413	GLU
1	A	423	ILE
1	A	446	LEU
1	A	504	CYS
1	A	511	VAL
1	A	571	GLN
1	A	574	ASP

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Mol	Chain	Res	Type
1	A	576	LYS
1	B	16	LEU
1	B	21	ARG
1	B	23	GLU
1	B	25	VAL
1	B	29	LEU
1	B	33	LYS
1	B	37	THR
1	B	40	LEU
1	B	51	LEU
1	B	52	LEU
1	B	64	GLU
1	B	72	GLN
1	B	98	THR
1	B	111	SER
1	B	122	SER
1	B	124	LEU
1	B	139	ASP
1	B	143	SER
1	B	157	ARG
1	B	187	SER
1	B	191	GLU
1	B	194	LYS
1	B	198	LEU
1	B	208	MET
1	B	212	LEU
1	B	218	ASP
1	B	250	GLN
1	B	256	SER
1	B	277	GLU
1	B	295	GLU
1	B	316	ASP
1	B	318	ARG
1	B	323	MET
1	B	327	LEU
1	B	360	ASN
1	B	381	ARG
1	B	398	ARG
1	B	405	LEU
1	B	410	GLU
1	B	418	ARG
1	B	427	MET

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Mol	Chain	Res	Type
1	B	441	GLU
1	B	460	GLU
1	B	465	ASN
1	B	466	LEU
1	B	468	LYS
1	B	479	HIS
1	B	481	THR
1	B	493	PRO
1	B	502	LEU
1	B	515	ASP
1	B	552	ASP
1	B	566	LYS
1	C	13	ILE
1	C	16	LEU
1	C	20	LEU
1	C	21	ARG
1	C	24	ASP
1	C	25	VAL
1	C	27	LEU
1	C	32	ILE
1	C	35	LEU
1	C	45	GLU
1	C	51	LEU
1	C	55	LEU
1	C	57	ASP
1	C	63	ASP
1	C	66	LEU
1	C	73	LEU
1	C	102	THR
1	C	140	TRP
1	C	145	THR
1	C	153	VAL
1	C	160	SER
1	C	175	SER
1	C	177	ASP
1	C	178	THR
1	C	189	LEU
1	C	191	GLU
1	C	198	LEU
1	C	202	LYS
1	C	218	ASP
1	C	222	LEU

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Mol	Chain	Res	Type
1	C	255	LYS
1	C	272	LYS
1	C	274	VAL
1	C	282	ASP
1	C	283	LEU
1	C	307	LYS
1	C	320	ASN
1	C	385	ILE
1	C	392	ASN
1	C	398	ARG
1	C	400	LEU
1	C	402	GLN
1	C	427	MET
1	C	448	MET
1	C	458	ILE
1	C	463	THR
1	C	464	SER
1	C	468	LYS
1	C	475	LYS
1	C	481	THR
1	C	506	ASN
1	C	539	ASN
1	C	555	THR
1	C	584	THR
1	D	16	LEU
1	D	21	ARG
1	D	25	VAL
1	D	27	LEU
1	D	32	ILE
1	D	34	LYS
1	D	37	THR
1	D	47	THR
1	D	66	LEU
1	D	67	LEU
1	D	75	THR
1	D	79	LEU
1	D	86	VAL
1	D	98	THR
1	D	102	THR
1	D	131	LEU
1	D	139	ASP
1	D	169	TYR

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Mol	Chain	Res	Type
1	D	192	PHE
1	D	194	LYS
1	D	216	GLU
1	D	222	LEU
1	D	248	LEU
1	D	266	LYS
1	D	271	GLN
1	D	280	LYS
1	D	290	LEU
1	D	313	LEU
1	D	316	ASP
1	D	320	ASN
1	D	345	LEU
1	D	370	LEU
1	D	376	GLU
1	D	382	LEU
1	D	385	ILE
1	D	389	ASP
1	D	395	ILE
1	D	397	ILE
1	D	400	LEU
1	D	403	SER
1	D	409	VAL
1	D	416	LYS
1	D	441	GLU
1	D	481	THR
1	D	498	ARG
1	D	515	ASP
1	D	547	ILE
1	D	583	LEU
1	D	584	THR
2	E	5	LEU
2	E	6	ASN
2	E	7	ARG
2	E	31	ARG
2	E	35	LEU
2	E	52	MET
2	E	53	LYS
2	E	54	LYS
2	E	62	MET
2	E	77	PHE
2	E	89	ASN

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Mol	Chain	Res	Type
2	E	97	CYS
2	E	106	LYS
2	E	107	MET
2	E	109	THR
2	E	131	ASP
2	E	134	VAL
2	E	146	MET
2	E	152	LEU
2	E	153	CYS
2	E	163	ILE
2	E	168	THR
2	F	7	ARG
2	F	21	ARG
2	F	31	ARG
2	F	35	LEU
2	F	52	MET
2	F	53	LYS
2	F	97	CYS
2	F	105	LYS
2	F	107	MET
2	F	110	ASN
2	F	112	ILE
2	F	113	CYS
2	F	115	LEU
2	F	117	LEU
2	F	118	LEU
2	F	126	LYS
2	F	131	ASP
2	F	136	VAL
2	F	152	LEU
2	F	153	CYS
2	F	159	LEU
2	F	163	ILE
2	F	164	ILE
2	F	168	THR
2	G	1	MET
2	G	5	LEU
2	G	6	ASN
2	G	7	ARG
2	G	19	LEU
2	G	31	ARG
2	G	52	MET

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Mol	Chain	Res	Type
2	G	53	LYS
2	G	54	LYS
2	G	63	GLU
2	G	64	ASP
2	G	100	TRP
2	G	107	MET
2	G	109	THR
2	G	112	ILE
2	G	113	CYS
2	G	114	LEU
2	G	115	LEU
2	G	120	MET
2	G	123	GLU
2	G	124	ASN
2	G	127	LEU
2	G	131	ASP
2	G	134	VAL
2	G	140	CYS
2	G	145	ARG
2	G	146	MET
2	G	152	LEU
2	G	153	CYS
2	G	157	LEU
2	G	159	LEU
2	G	163	ILE
2	G	171	ASP
2	H	1	MET
2	H	2	ASP
2	H	6	ASN
2	H	21	ARG
2	H	52	MET
2	H	58	LEU
2	H	62	MET
2	H	67	LYS
2	H	70	HIS
2	H	105	LYS
2	H	109	THR
2	H	111	CYS
2	H	115	LEU
2	H	119	ARG
2	H	124	ASN
2	H	127	LEU

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Mol	Chain	Res	Type
2	H	129	ARG
2	H	131	ASP
2	H	136	VAL
2	H	142	ASP
2	H	170	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	117	HIS
1	A	119	HIS
1	A	217	GLN
1	A	250	GLN
1	A	271	GLN
1	A	288	GLN
1	A	320	ASN
1	A	325	GLN
1	A	338	ASN
1	A	387	ASN
1	A	465	ASN
1	A	506	ASN
1	A	520	HIS
1	A	571	GLN
1	B	26	GLN
1	B	30	ASN
1	B	72	GLN
1	B	217	GLN
1	B	230	ASN
1	B	237	GLN
1	B	250	GLN
1	B	271	GLN
1	B	289	ASN
1	B	325	GLN
1	B	338	ASN
1	B	340	HIS
1	B	392	ASN
1	B	402	GLN
1	B	444	ASN
1	B	506	ASN
1	B	514	GLN
1	B	520	HIS

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Mol	Chain	Res	Type
1	B	545	GLN
1	B	580	GLN
1	C	22	ASN
1	C	119	HIS
1	C	172	ASN
1	C	230	ASN
1	C	271	GLN
1	C	289	ASN
1	C	338	ASN
1	C	444	ASN
1	C	454	HIS
1	C	465	ASN
1	C	506	ASN
1	C	545	GLN
1	C	557	GLN
1	D	119	HIS
1	D	168	GLN
1	D	230	ASN
1	D	288	GLN
1	D	289	ASN
1	D	360	ASN
1	D	454	HIS
1	D	465	ASN
1	D	535	ASN
2	E	6	ASN
2	E	110	ASN
2	F	110	ASN
2	G	6	ASN
2	G	12	GLN
2	G	99	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	575/589 (97%)	-0.19	1 (0%) 93 61	98, 114, 132, 146	0
1	B	575/589 (97%)	-0.21	0 100 100	96, 112, 123, 132	0
1	C	577/589 (97%)	-0.05	7 (1%) 75 20	98, 114, 131, 135	0
1	D	577/589 (97%)	0.01	12 (2%) 60 11	98, 113, 140, 146	0
2	E	163/174 (93%)	-0.29	0 100 100	103, 113, 123, 133	0
2	F	152/174 (87%)	-0.15	2 (1%) 74 19	103, 114, 127, 136	0
2	G	142/174 (81%)	-0.18	1 (0%) 84 32	99, 114, 121, 125	0
2	H	143/174 (82%)	-0.16	1 (0%) 84 32	96, 112, 121, 127	0
All	All	2904/3052 (95%)	-0.13	24 (0%) 83 28	96, 113, 133, 146	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	544	LEU	4.3
1	D	512	CYS	4.3
2	F	49	GLU	4.0
1	D	586	LEU	3.7
1	C	504	CYS	3.6
1	C	589	ALA	3.4
1	C	434	LEU	2.8
1	D	557	GLN	2.7
1	D	496	LEU	2.7
1	D	550	ILE	2.7
2	H	107	MET	2.7
1	C	505	ILE	2.6
2	F	50	GLU	2.5
1	D	398	ARG	2.5
1	D	549	PRO	2.5
1	C	398	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	G	1	MET	2.4
1	C	559	GLU	2.4
1	A	442	LYS	2.4
1	D	521	MET	2.3
1	D	538	PHE	2.3
1	C	467	LYS	2.2
1	D	537	ARG	2.2
1	D	578	PHE	2.1

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 carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ZN	H	902	1/1	0.22	1.67	98,98,98,98	0
3	ZN	F	702	1/1	0.21	1.20	100,100,100,100	0
3	ZN	E	602	1/1	0.18	1.17	99,99,99,99	0
3	ZN	E	601	1/1	0.17	0.43	103,103,103,103	0
3	ZN	G	801	1/1	0.14	0.25	108,108,108,108	0
3	ZN	G	802	1/1	0.18	0.20	98,98,98,98	0
3	ZN	F	701	1/1	0.16	-0.46	108,108,108,108	0
3	ZN	H	901	1/1	0.11	-0.63	101,101,101,101	0

6.5 Other polymers ⓘ

There are no such residues in this entry.