



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:33 PM UTC

PDB ID : 4ZP4 / pdb_00004zp4
Title : Crystal Structure of the Heterodimeric HIF-2 α :ARNT Complex
Authors : Wu, D.; Potluri, N.; Lu, J.; Kim, Y.; Rastinejad, F.
Deposited on : 2015-05-07
Resolution : 2.35 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

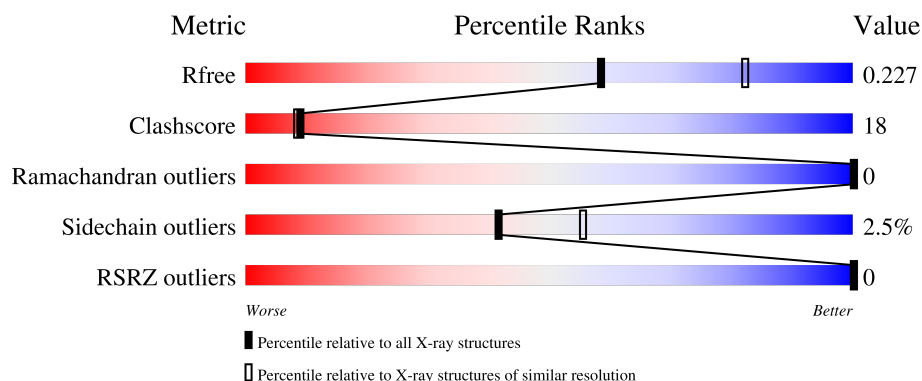
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

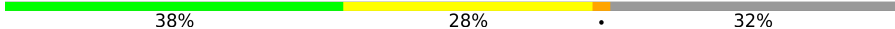
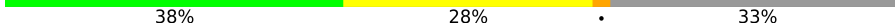
The reported resolution of this entry is 2.35 Å.

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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	384	
1	C	384	
2	B	360	
2	D	360	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9063 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 Aryl hydrocarbon receptor nuclear translocator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2124	1348	374	386	16			
1	C	258	Total	C	N	O	S	0	0	0
			2101	1332	371	382	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	MET	-	initiating methionine	UNP P53762
C	81	MET	-	initiating methionine	UNP P53762

- Molecule 2 is a protein called Endothelial PAS domain-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	295	Total	C	N	O	S	0	0	0
			2374	1498	408	444	24			
2	D	288	Total	C	N	O	S	0	0	0
			2325	1474	394	435	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	MET	-	initiating methionine	UNP P97481
D	2	MET	-	initiating methionine	UNP P97481

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total	O	0	0
			28	28		
3	B	35	Total	O	0	0
			35	35		

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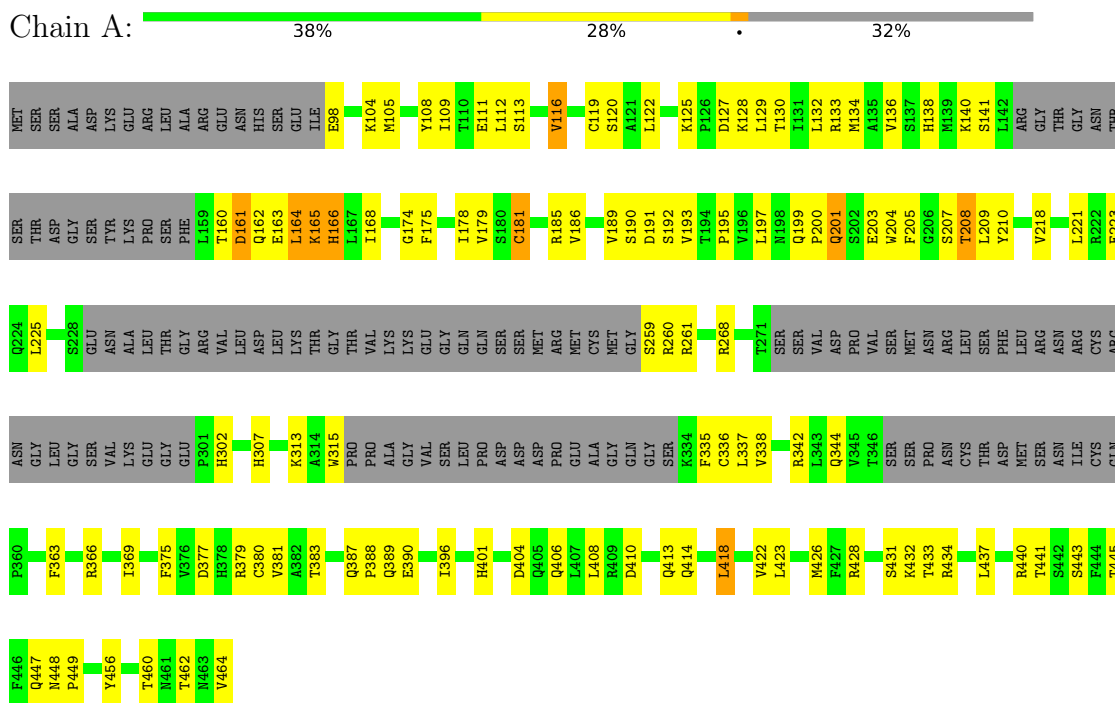
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	32	Total 32	O 32	0	0
3	D	44	Total 44	O 44	0	0

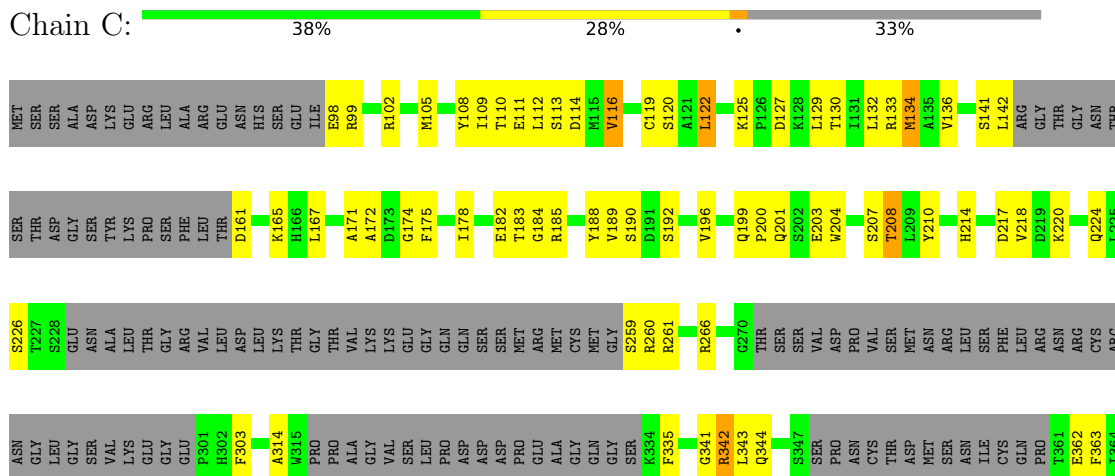
3 Residue-property plots

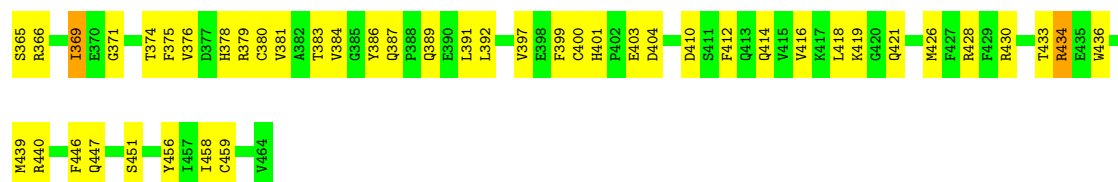
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Aryl hydrocarbon receptor nuclear translocator



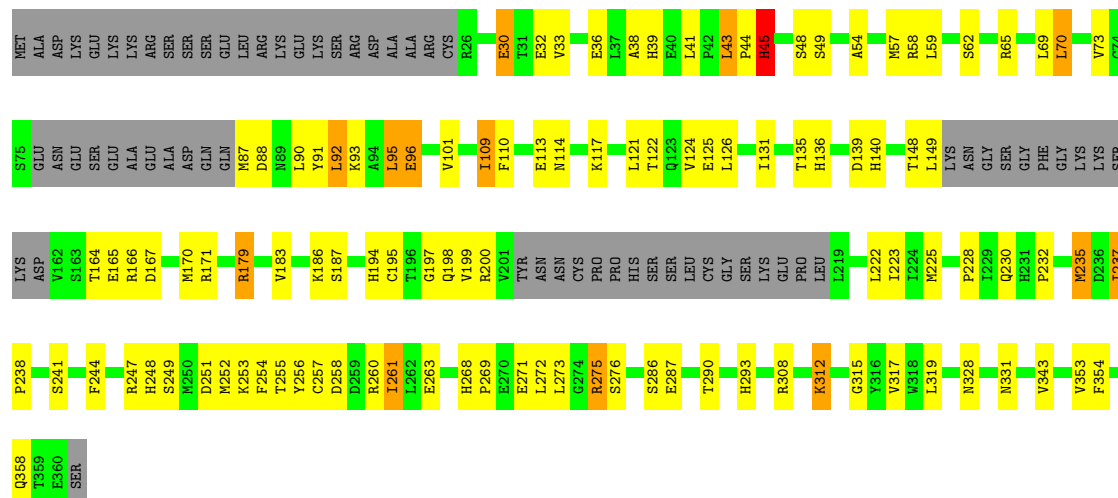
- Molecule 1: Aryl hydrocarbon receptor nuclear translocator





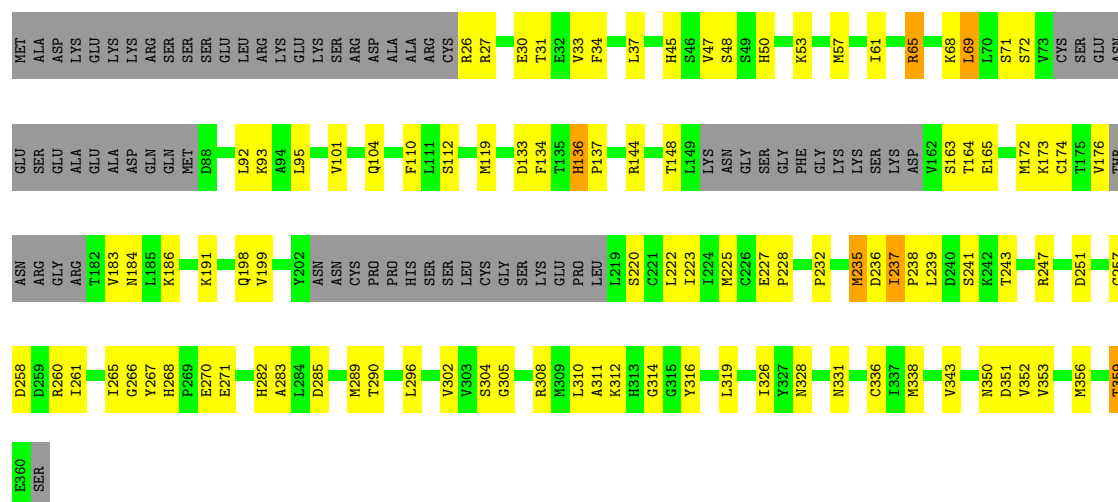
• Molecule 2: Endothelial PAS domain-containing protein 1

Chain B: 51% 27% 18%



• Molecule 2: Endothelial PAS domain-containing protein 1

Chain D: 52% 26% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.01Å 76.46Å 98.82Å 90.06° 90.19° 73.13°	Depositor
Resolution (Å)	49.41 – 2.35 49.41 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.41-2.35) 97.4 (49.41-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.37Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.200 , 0.232 0.207 , 0.227	Depositor DCC
R_{free} test set	2827 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	55.0	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 76.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,h-k,-l 0.448 for -h,-k,l 0.018 for -h,-h+k,-l	Xtriage
Reported twinning fraction	0.470 for -h,-k,l	Depositor
Outliers	0 of 55771 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9063	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.70	0/2166	1.08	7/2920 (0.2%)
1	C	0.70	0/2142	1.06	11/2886 (0.4%)
2	B	0.72	0/2421	1.08	14/3265 (0.4%)
2	D	0.74	0/2372	1.07	10/3200 (0.3%)
All	All	0.71	0/9101	1.07	42/12271 (0.3%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	237	ILE	CA-C-N	11.76	131.90	119.90
2	D	237	ILE	C-N-CA	11.76	131.90	119.90
2	B	237	ILE	CA-C-N	10.76	130.87	119.90
2	B	237	ILE	C-N-CA	10.76	130.87	119.90
2	B	45	HIS	N-CA-C	-9.09	101.38	111.28
2	B	237	ILE	N-CA-C	8.32	117.86	108.05
1	C	134	MET	N-CA-C	-7.83	102.64	112.90
1	A	201	GLN	N-CA-C	-7.59	102.98	111.71
2	B	179	ARG	N-CA-C	7.09	121.43	111.92
1	C	184	GLY	N-CA-C	-6.95	105.63	115.43
2	B	96	GLU	N-CA-C	-6.95	104.12	112.59
2	B	186	LYS	N-CA-C	-6.75	104.86	113.23
1	A	140	LYS	N-CA-C	-6.33	104.82	112.54
2	D	359	THR	N-CA-C	6.12	117.95	111.28
2	D	305	GLY	N-CA-C	-6.03	102.90	112.66
2	B	49	SER	N-CA-C	5.92	119.61	112.38
2	D	235	MET	N-CA-C	5.87	118.29	108.02
2	B	235	MET	N-CA-C	5.75	118.08	108.02
1	A	116	VAL	CA-C-N	5.74	124.93	118.97
1	A	116	VAL	C-N-CA	5.74	124.93	118.97
1	A	401	HIS	CA-C-N	5.68	126.94	119.84
1	A	401	HIS	C-N-CA	5.68	126.94	119.84
2	D	136	HIS	CA-C-N	5.67	126.05	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	136	HIS	C-N-CA	5.67	126.05	119.47
1	C	362	GLU	N-CA-C	5.63	116.82	108.60
1	C	125	LYS	CA-C-N	5.60	125.59	120.21
1	C	125	LYS	C-N-CA	5.60	125.59	120.21
2	B	136	HIS	CA-C-N	5.57	125.93	119.47
2	B	136	HIS	C-N-CA	5.57	125.93	119.47
1	A	181	CYS	N-CA-C	5.53	117.39	111.36
1	C	122	LEU	N-CA-C	5.51	119.09	110.32
1	C	127	ASP	N-CA-C	5.43	117.54	110.53
2	B	70	LEU	N-CA-C	5.39	117.16	111.28
2	B	255	THR	N-CA-C	-5.39	106.63	114.12
2	D	69	LEU	N-CA-C	-5.39	105.41	111.28
1	C	218	VAL	N-CA-C	5.14	115.35	110.42
1	C	226	SER	N-CA-C	5.12	118.11	110.52
2	D	65	ARG	N-CA-C	-5.12	105.70	111.28
2	B	43	LEU	N-CA-C	5.11	114.17	108.25
1	C	116	VAL	CA-C-N	5.10	124.27	118.97
1	C	116	VAL	C-N-CA	5.10	124.27	118.97
2	D	237	ILE	N-CA-C	5.04	113.39	107.89

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2124	0	2118	99	0
1	C	2101	0	2090	91	0
2	B	2374	0	2341	87	0
2	D	2325	0	2288	84	0
3	A	28	0	0	1	0
3	B	35	0	0	0	0
3	C	32	0	0	0	0
3	D	44	0	0	0	0
All	All	9063	0	8837	327	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 (327) 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:163:GLU:HG2	2:B:70:LEU:HD12	1.29	1.12
1:A:160:THR:HB	1:A:163:GLU:HB2	1.45	0.96
1:A:315:TRP:CD1	1:A:336:CYS:HG	1.93	0.86
1:A:164:LEU:O	1:A:164:LEU:HD12	1.79	0.82
2:D:266:GLY:HA3	2:D:312:LYS:HG2	1.63	0.80
2:B:54:ALA:O	2:B:58:ARG:HG3	1.88	0.73
2:D:241:SER:HA	2:D:260:ARG:HH11	1.55	0.70
1:A:189:VAL:HG11	1:A:204:TRP:HB3	1.74	0.70
1:C:428:ARG:HB3	1:C:436:TRP:HB3	1.74	0.70
2:D:239:LEU:HD13	2:D:243:THR:HG21	1.73	0.70
1:C:132:LEU:O	1:C:136:VAL:HG23	1.92	0.69
2:D:232:PRO:HA	2:D:235:MET:HE3	1.73	0.69
1:A:207:SER:OG	1:A:208:THR:N	2.25	0.68
2:B:87:MET:HE3	2:B:90:LEU:HD12	1.76	0.68
1:A:181:CYS:HB2	1:A:335:PHE:HB2	1.75	0.68
1:C:387:GLN:HB3	1:C:389:GLN:OE1	1.94	0.68
1:A:377:ASP:OD2	1:A:379:ARG:NH2	2.23	0.67
1:A:440:ARG:NH2	1:A:462:THR:OG1	2.27	0.67
1:C:172:ALA:HB1	1:C:342:ARG:HD3	1.77	0.67
1:A:390:GLU:OE2	1:A:432:LYS:NZ	2.21	0.65
1:C:386:TYR:OH	1:C:430:ARG:NH1	2.28	0.65
2:D:165:GLU:CD	2:D:198:GLN:HE22	2.05	0.65
1:A:164:LEU:HD12	1:A:164:LEU:C	2.21	0.64
1:A:315:TRP:HB3	1:A:336:CYS:HB2	1.78	0.64
2:B:269:PRO:O	2:B:273:LEU:HG	1.97	0.64
2:D:164:THR:OG1	2:D:198:GLN:NE2	2.31	0.64
2:D:101:VAL:HB	2:D:110:PHE:HB3	1.79	0.63
1:C:110:THR:O	1:C:113:SER:OG	2.14	0.63
1:A:105:MET:O	1:A:109:ILE:HG12	1.97	0.63
2:B:131:ILE:HD11	2:B:170:MET:HE1	1.79	0.63
1:A:313:LYS:HG3	1:A:313:LYS:O	1.99	0.62
1:C:260:ARG:NH2	2:D:93:LYS:O	2.31	0.62
1:C:399:PHE:O	1:C:430:ARG:N	2.30	0.62
1:C:433:THR:O	1:C:434:ARG:HB2	2.00	0.62
1:A:175:PHE:HB2	1:A:192:SER:HB2	1.81	0.62
2:D:174:CYS:SG	2:D:191:LYS:HE2	2.40	0.62
2:B:135:THR:O	2:B:140:HIS:NE2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:165:GLU:N	2:D:165:GLU:OE1	2.32	0.61
2:B:179:ARG:O	2:B:179:ARG:HG2	2.01	0.61
2:B:268:HIS:HB2	2:B:271:GLU:HG3	1.83	0.61
1:C:381:VAL:HG22	1:C:387:GLN:HA	1.83	0.60
1:C:366:ARG:HB2	1:C:375:PHE:HB3	1.83	0.60
1:A:406:GLN:O	1:A:410:ASP:N	2.31	0.60
1:A:426:MET:HE3	1:A:464:VAL:HG21	1.82	0.60
2:B:41:LEU:O	2:B:43:LEU:N	2.35	0.59
1:A:223:GLU:OE2	2:B:241:SER:OG	2.20	0.59
1:A:161:ASP:HA	2:B:88:ASP:OD2	2.03	0.59
2:D:61:ILE:HG22	2:D:65:ARG:HD2	1.84	0.59
2:D:104:GLN:HB3	2:D:220:SER:H	1.67	0.59
2:D:95:LEU:HD22	2:D:225:MET:HE3	1.85	0.59
1:A:191:ASP:OD1	1:A:191:ASP:N	2.27	0.58
1:C:404:ASP:OD1	1:C:428:ARG:NH2	2.31	0.58
1:A:389:GLN:HG3	2:B:353:VAL:HG21	1.86	0.58
1:C:105:MET:O	1:C:109:ILE:HG12	2.03	0.58
2:B:287:GLU:O	2:B:290:THR:OG1	2.15	0.58
2:D:268:HIS:N	2:D:271:GLU:OE2	2.23	0.58
2:D:326:ILE:HG13	2:D:338:MET:HG2	1.84	0.58
2:B:232:PRO:HA	2:B:235:MET:HE3	1.86	0.58
1:A:179:VAL:HG12	1:A:186:VAL:HG22	1.86	0.58
1:C:189:VAL:O	1:C:201:GLN:NE2	2.33	0.58
1:A:132:LEU:HB3	2:B:33:VAL:HG21	1.84	0.57
2:B:32:GLU:O	2:B:36:GLU:HG3	2.03	0.57
1:A:116:VAL:HB	1:A:119:CYS:HB3	1.85	0.57
1:A:160:THR:HG22	1:A:162:GLN:H	1.68	0.57
1:C:342:ARG:HH12	1:C:344:GLN:HB2	1.70	0.57
1:C:446:PHE:HZ	2:D:290:THR:HB	1.69	0.57
2:D:289:MET:HE1	2:D:304:SER:HB2	1.86	0.57
2:D:199:VAL:HG22	2:D:222:LEU:HD13	1.86	0.57
1:A:210:TYR:CD1	1:A:218:VAL:HG13	2.39	0.57
1:A:387:GLN:N	1:A:390:GLU:OE1	2.25	0.57
1:C:214:HIS:HB2	1:C:266:ARG:HB2	1.85	0.57
2:B:101:VAL:HG13	2:B:109:ILE:CD1	2.34	0.56
2:D:296:LEU:HD13	2:D:302:VAL:HG22	1.87	0.56
1:A:128:LYS:HD3	2:B:30:GLU:CD	2.29	0.56
1:A:380:CYS:SG	1:A:381:VAL:N	2.78	0.56
2:D:268:HIS:HB3	2:D:270:GLU:OE1	2.05	0.56
1:A:163:GLU:HG2	2:B:70:LEU:CD1	2.21	0.56
1:A:389:GLN:OE1	1:A:389:GLN:N	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:HIS:O	1:A:141:SER:HB3	2.05	0.56
1:A:189:VAL:HG13	1:A:201:GLN:HG3	1.88	0.56
1:C:200:PRO:HG2	1:C:203:GLU:HB2	1.88	0.56
1:C:426:MET:HG2	1:C:440:ARG:HB2	1.88	0.56
2:D:241:SER:C	2:D:243:THR:H	2.14	0.56
1:C:141:SER:OG	1:C:142:LEU:N	2.39	0.56
2:D:34:PHE:CD2	2:D:53:LYS:HD3	2.40	0.56
1:A:113:SER:O	1:A:120:SER:HB2	2.06	0.55
2:B:114:ASN:O	2:B:117:LYS:HB3	2.07	0.55
1:A:313:LYS:HG2	1:A:338:VAL:CG2	2.37	0.55
2:D:31:THR:HG22	2:D:53:LYS:NZ	2.21	0.55
1:A:379:ARG:O	1:A:383:THR:HG23	2.07	0.55
1:C:130:THR:O	1:C:133:ARG:N	2.40	0.55
2:D:328:ASN:HB3	2:D:331:ASN:OD1	2.07	0.55
1:C:261:ARG:HG3	2:D:238:PRO:HG2	1.88	0.55
1:A:130:THR:O	1:A:133:ARG:N	2.40	0.54
1:C:111:GLU:HA	1:C:114:ASP:OD2	2.08	0.54
1:A:201:GLN:O	1:A:205:PHE:N	2.29	0.54
2:B:286:SER:O	2:B:290:THR:HG23	2.08	0.54
2:B:101:VAL:HG12	2:B:110:PHE:HB3	1.90	0.54
2:B:354:PHE:N	2:B:358:GLN:OE1	2.35	0.54
2:D:134:PHE:HA	2:D:173:LYS:HD2	1.90	0.54
2:B:58:ARG:O	2:B:62:SER:OG	2.19	0.54
2:D:199:VAL:CG2	2:D:222:LEU:HD13	2.38	0.54
2:B:319:LEU:HD23	2:B:343:VAL:HA	1.89	0.54
1:C:397:VAL:O	1:C:400:CYS:HB3	2.07	0.54
1:A:313:LYS:HG2	1:A:338:VAL:HG23	1.88	0.53
1:C:161:ASP:N	1:C:161:ASP:OD1	2.41	0.53
2:B:139:ASP:CG	2:B:171:ARG:HH21	2.15	0.53
2:D:241:SER:HA	2:D:260:ARG:NH1	2.23	0.53
2:B:92:LEU:HD21	2:B:113:GLU:HB3	1.90	0.53
1:C:129:LEU:O	1:C:133:ARG:HG3	2.08	0.53
1:C:112:LEU:HD22	2:D:57:MET:HE1	1.90	0.53
2:B:122:THR:OG1	2:B:125:GLU:HG3	2.09	0.53
1:A:388:PRO:HB2	2:B:353:VAL:HG23	1.91	0.53
1:C:378:HIS:HB2	2:D:352:VAL:HG11	1.92	0.52
1:C:401:HIS:ND1	1:C:403:GLU:HG2	2.25	0.52
1:A:116:VAL:O	1:A:120:SER:N	2.32	0.52
1:C:266:ARG:HB3	1:C:303:PHE:HB3	1.91	0.52
1:C:366:ARG:HH21	2:D:283:ALA:HA	1.73	0.52
2:D:258:ASP:O	2:D:261:ILE:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:351:ASP:OD1	2:D:351:ASP:N	2.42	0.52
2:D:356:MET:O	2:D:359:THR:OG1	2.26	0.52
2:B:38:ALA:O	2:B:48:SER:HB2	2.10	0.51
1:C:185:ARG:HD3	1:C:207:SER:O	2.11	0.51
2:D:163:SER:OG	2:D:165:GLU:OE1	2.26	0.51
1:A:380:CYS:HA	1:A:383:THR:OG1	2.11	0.51
2:B:260:ARG:HA	2:B:263:GLU:OE1	2.11	0.51
1:A:445:THR:HG22	1:A:447:GLN:NE2	2.25	0.51
2:B:247:ARG:HG2	2:B:248:HIS:N	2.24	0.51
1:C:418:LEU:HB3	1:C:421:GLN:OE1	2.11	0.51
2:D:247:ARG:HD2	2:D:336:CYS:SG	2.51	0.50
1:A:129:LEU:O	1:A:133:ARG:HG3	2.11	0.50
2:B:101:VAL:HA	2:B:222:LEU:O	2.11	0.50
1:A:122:LEU:HD11	1:A:134:MET:HE1	1.92	0.50
1:A:179:VAL:HG12	1:A:186:VAL:HA	1.94	0.50
1:A:193:VAL:HG23	1:A:197:LEU:HD12	1.93	0.50
1:A:414:GLN:HG3	1:A:418:LEU:HD13	1.93	0.50
1:C:381:VAL:HA	1:C:386:TYR:O	2.12	0.50
2:B:148:THR:O	2:B:166:ARG:NH2	2.43	0.50
1:C:175:PHE:HB2	1:C:192:SER:HB2	1.94	0.50
1:A:165:LYS:HB2	2:B:91:TYR:CZ	2.47	0.50
2:D:184:ASN:ND2	2:D:186:LYS:HB3	2.27	0.50
2:D:69:LEU:O	2:D:72:SER:HB3	2.12	0.49
2:D:92:LEU:HD21	2:D:112:SER:HB2	1.94	0.49
1:A:132:LEU:HB3	2:B:33:VAL:CG2	2.41	0.49
1:C:130:THR:O	1:C:134:MET:HG3	2.12	0.49
2:B:62:SER:HB3	2:B:109:ILE:O	2.13	0.49
1:C:108:TYR:HB3	2:D:57:MET:HB3	1.93	0.49
2:D:47:VAL:HG23	2:D:48:SER:N	2.28	0.49
1:C:116:VAL:O	1:C:120:SER:N	2.43	0.49
1:C:178:ILE:HD12	1:C:188:TYR:HB3	1.95	0.48
2:D:45:HIS:HA	2:D:48:SER:OG	2.13	0.48
2:D:164:THR:CB	2:D:198:GLN:HE21	2.25	0.48
2:B:101:VAL:HG13	2:B:109:ILE:HD11	1.95	0.48
1:A:130:THR:O	1:A:134:MET:HG3	2.13	0.48
1:A:132:LEU:O	1:A:136:VAL:HG23	2.14	0.48
2:B:315:GLY:HA2	2:B:354:PHE:HE1	1.79	0.48
1:C:172:ALA:HB1	1:C:342:ARG:CD	2.43	0.48
2:B:38:ALA:O	2:B:41:LEU:HB2	2.14	0.48
1:C:389:GLN:CG	2:D:353:VAL:HB	2.44	0.48
1:C:129:LEU:HD11	2:D:30:GLU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:LEU:C	2:B:166:ARG:HH22	2.22	0.47
1:A:111:GLU:OE2	2:B:65:ARG:NH2	2.46	0.47
2:B:87:MET:HB2	2:B:90:LEU:HD12	1.94	0.47
2:B:197:GLY:HA3	2:B:223:ILE:O	2.14	0.47
1:C:217:ASP:O	1:C:220:LYS:HG2	2.15	0.47
1:A:120:SER:C	1:A:122:LEU:H	2.21	0.47
1:A:413:GLN:HA	2:D:50:HIS:ND1	2.30	0.47
1:C:314:ALA:HA	1:C:335:PHE:HA	1.96	0.47
2:D:258:ASP:OD2	2:D:260:ARG:HB2	2.13	0.47
1:C:451:SER:HB3	2:D:251:ASP:HB3	1.97	0.47
1:A:445:THR:CG2	1:A:447:GLN:NE2	2.78	0.47
2:B:252:MET:HG2	2:B:293:HIS:NE2	2.30	0.47
1:C:99:ARG:HB2	1:C:102:ARG:HH21	1.80	0.47
2:D:164:THR:N	2:D:165:GLU:OE1	2.48	0.47
1:A:130:THR:HG22	1:A:134:MET:CG	2.44	0.47
1:A:200:PRO:HB2	1:A:203:GLU:H	1.80	0.47
1:C:456:TYR:HE1	1:C:458:ILE:HD11	1.79	0.47
2:D:237:ILE:HA	2:D:238:PRO:HD2	1.53	0.47
1:A:259:SER:HB2	1:A:261:ARG:HH21	1.80	0.47
2:B:69:LEU:CD2	2:B:101:VAL:HG21	2.45	0.47
1:A:366:ARG:HD2	1:A:456:TYR:CE1	2.50	0.46
1:C:119:CYS:HA	1:C:122:LEU:HG	1.95	0.46
1:C:434:ARG:HA	1:C:434:ARG:HD3	1.59	0.46
1:A:189:VAL:HG22	1:A:190:SER:O	2.15	0.46
2:D:26:ARG:HD2	2:D:27:ARG:H	1.79	0.46
1:A:105:MET:O	1:A:108:TYR:HB2	2.16	0.46
1:C:414:GLN:O	1:C:418:LEU:N	2.37	0.46
1:A:431:SER:HB3	1:A:437:LEU:HD11	1.98	0.46
1:C:175:PHE:HE2	1:C:189:VAL:HG23	1.81	0.46
2:B:44:PRO:O	2:B:45:HIS:C	2.57	0.46
2:B:328:ASN:HB3	2:B:331:ASN:OD1	2.16	0.46
1:A:366:ARG:HD2	1:A:456:TYR:CZ	2.51	0.46
1:C:369:ILE:H	1:C:369:ILE:HG13	1.59	0.46
2:B:96:GLU:O	2:B:228:PRO:HD2	2.16	0.45
2:D:68:LYS:O	2:D:71:SER:HB3	2.16	0.45
2:B:32:GLU:HG2	2:B:36:GLU:OE2	2.16	0.45
1:C:132:LEU:HB3	2:D:33:VAL:HG22	1.98	0.45
1:A:132:LEU:HD13	2:B:33:VAL:HG13	1.98	0.45
2:D:136:HIS:HA	2:D:137:PRO:HD3	1.85	0.45
1:A:160:THR:HG22	1:A:162:GLN:N	2.30	0.45
1:A:192:SER:HA	1:A:195:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:ARG:HB3	2:B:256:TYR:HB3	1.98	0.45
1:C:136:VAL:HG22	2:D:37:LEU:HA	1.97	0.45
2:B:230:GLN:NE2	2:B:237:ILE:HD12	2.31	0.45
2:B:252:MET:HG2	2:B:293:HIS:CE1	2.52	0.45
1:C:178:ILE:HD12	1:C:188:TYR:HD2	1.81	0.45
1:C:342:ARG:NH1	1:C:343:LEU:O	2.48	0.45
1:C:389:GLN:HG3	2:D:353:VAL:HB	1.98	0.45
1:C:447:GLN:N	1:C:447:GLN:OE1	2.49	0.45
1:A:426:MET:HE2	1:A:426:MET:HB3	1.86	0.45
1:C:167:LEU:HD23	1:C:167:LEU:HA	1.83	0.45
1:A:165:LYS:HB2	2:B:91:TYR:CE2	2.52	0.45
2:B:308:ARG:HA	2:B:317:VAL:O	2.16	0.45
2:D:61:ILE:O	2:D:65:ARG:HG3	2.15	0.45
2:D:326:ILE:HB	2:D:336:CYS:SG	2.56	0.45
1:A:127:ASP:OD1	1:A:130:THR:OG1	2.14	0.45
2:D:265:ILE:HG22	2:D:267:TYR:CE2	2.51	0.45
2:D:319:LEU:HD23	2:D:343:VAL:HA	1.98	0.45
2:B:165:GLU:HA	2:B:198:GLN:HG3	1.98	0.45
2:D:34:PHE:CE1	2:D:53:LYS:HB3	2.52	0.45
1:A:268:ARG:HA	1:A:302:HIS:O	2.17	0.44
2:B:121:LEU:HD13	2:B:126:LEU:HD21	1.99	0.44
2:B:167:ASP:OD1	2:B:194:HIS:NE2	2.50	0.44
1:A:160:THR:HB	1:A:163:GLU:CB	2.33	0.44
1:C:383:THR:HG22	1:C:384:VAL:HG13	1.99	0.44
1:C:416:VAL:O	1:C:419:LYS:HG3	2.17	0.44
1:A:125:LYS:H	1:A:125:LYS:HG3	1.57	0.44
1:A:448:ASN:HA	1:A:449:PRO:HD3	1.83	0.44
2:B:271:GLU:OE2	2:B:312:LYS:NZ	2.51	0.44
1:C:208:THR:HG22	1:C:210:TYR:H	1.82	0.44
1:C:376:VAL:HG21	1:C:391:LEU:HB2	1.98	0.44
1:C:410:ASP:O	1:C:414:GLN:HG2	2.18	0.44
1:A:181:CYS:N	1:A:335:PHE:O	2.44	0.44
2:B:73:VAL:HG22	2:B:200:ARG:CZ	2.48	0.44
2:B:257:CYS:SG	2:B:261:ILE:HD13	2.58	0.44
2:B:54:ALA:O	2:B:57:MET:HB2	2.17	0.44
2:D:37:LEU:HA	2:D:37:LEU:HD12	1.79	0.44
2:D:236:ASP:N	2:D:236:ASP:OD1	2.45	0.44
1:A:307:HIS:HE1	1:A:344:GLN:OE1	2.01	0.44
1:C:171:ALA:HB2	2:D:223:ILE:HG22	2.00	0.44
2:D:34:PHE:CE2	2:D:53:LYS:HD3	2.53	0.44
1:A:344:GLN:NE2	3:A:503:HOH:O	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:272:LEU:C	2:B:275:ARG:HG3	2.42	0.44
1:A:163:GLU:HA	1:A:166:HIS:HB2	2.00	0.43
1:A:404:ASP:OD2	1:A:428:ARG:HD2	2.18	0.43
1:C:380:CYS:SG	1:C:381:VAL:N	2.90	0.43
2:B:38:ALA:HA	2:B:41:LEU:HD12	2.00	0.43
1:C:132:LEU:HB3	2:D:33:VAL:CG2	2.48	0.43
2:D:165:GLU:CG	2:D:198:GLN:HE22	2.31	0.43
1:A:193:VAL:HG22	1:A:199:GLN:HB3	2.01	0.43
1:A:389:GLN:H	1:A:389:GLN:CD	2.13	0.43
1:A:363:PHE:HB2	1:A:377:ASP:OD1	2.18	0.43
2:D:101:VAL:HG23	2:D:110:PHE:HD2	1.84	0.43
2:D:144:ARG:O	2:D:148:THR:HG23	2.18	0.43
1:A:260:ARG:NH1	2:B:93:LYS:O	2.30	0.43
2:B:249:SER:OG	2:B:251:ASP:OD1	2.24	0.43
1:A:178:ILE:HA	1:A:337:LEU:O	2.18	0.43
2:B:101:VAL:CG1	2:B:109:ILE:HD11	2.49	0.43
1:A:363:PHE:HB3	1:A:383:THR:HG21	2.01	0.43
1:A:375:PHE:HA	2:B:354:PHE:O	2.19	0.43
2:B:258:ASP:O	2:B:261:ILE:HG22	2.18	0.43
1:C:376:VAL:HG11	1:C:391:LEU:HD12	2.00	0.43
1:A:174:GLY:HA2	1:A:342:ARG:HA	2.01	0.43
1:C:189:VAL:HG13	1:C:201:GLN:HG3	1.99	0.43
1:C:446:PHE:CZ	2:D:290:THR:HB	2.51	0.43
2:B:95:LEU:HD12	2:B:95:LEU:HA	1.84	0.42
2:D:227:GLU:HA	2:D:228:PRO:HD2	1.91	0.42
1:C:259:SER:CB	1:C:261:ARG:HH12	2.31	0.42
2:D:119:MET:HE2	2:D:172:MET:SD	2.59	0.42
1:A:199:GLN:HG2	1:A:204:TRP:HE1	1.84	0.42
1:C:182:GLU:HG2	1:C:183:THR:HG23	2.01	0.42
2:D:31:THR:HG22	2:D:53:LYS:HZ3	1.84	0.42
2:D:183:VAL:HG12	2:D:184:ASN:N	2.34	0.42
1:A:112:LEU:HA	1:A:112:LEU:HD23	1.81	0.42
1:C:365:SER:OG	1:C:459:CYS:HB2	2.19	0.42
1:A:433:THR:O	1:A:434:ARG:HB2	2.19	0.42
2:B:170:MET:HG2	2:B:195:CYS:SG	2.60	0.42
1:C:426:MET:HA	1:C:439:MET:O	2.19	0.42
1:C:189:VAL:HG22	1:C:190:SER:O	2.19	0.42
1:C:208:THR:CG2	1:C:210:TYR:HD2	2.32	0.42
1:A:130:THR:O	1:A:134:MET:N	2.53	0.42
1:C:174:GLY:HA2	1:C:341:GLY:O	2.20	0.42
1:C:371:GLY:HA2	1:C:412:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:HIS:HA	2:B:253:LYS:O	2.19	0.42
1:C:363:PHE:HB2	1:C:379:ARG:HG3	2.00	0.42
2:D:283:ALA:C	2:D:285:ASP:H	2.27	0.42
1:A:423:LEU:HD12	1:A:423:LEU:HA	1.75	0.42
2:B:195:CYS:HA	2:B:225:MET:O	2.19	0.42
2:B:101:VAL:CG1	2:B:109:ILE:CD1	2.97	0.41
1:A:441:THR:HA	1:A:460:THR:O	2.20	0.41
2:B:165:GLU:CD	2:B:198:GLN:HE21	2.27	0.41
2:B:237:ILE:HA	2:B:238:PRO:HD2	1.56	0.41
2:D:314:GLY:HA3	2:D:350:ASN:O	2.20	0.41
1:C:132:LEU:HD23	1:C:132:LEU:HA	1.90	0.41
1:C:174:GLY:HA3	1:C:342:ARG:HB3	2.02	0.41
1:A:160:THR:HG22	1:A:161:ASP:N	2.35	0.41
2:D:310:LEU:HD23	2:D:316:TYR:HB3	2.01	0.41
2:B:253:LYS:HA	2:B:276:SER:HA	2.03	0.41
1:C:220:LYS:O	1:C:224:GLN:HG2	2.21	0.41
1:C:374:THR:HA	2:D:356:MET:HG3	2.02	0.41
1:A:422:VAL:HA	1:A:443:SER:O	2.21	0.41
1:C:136:VAL:HG22	2:D:37:LEU:CA	2.51	0.41
2:B:254:PHE:HB2	2:B:272:LEU:O	2.20	0.41
1:C:418:LEU:O	1:C:421:GLN:HG3	2.20	0.41
2:D:257:CYS:SG	2:D:261:ILE:HB	2.61	0.41
1:C:192:SER:O	1:C:196:VAL:HG23	2.21	0.41
1:A:221:LEU:O	1:A:225:LEU:HD13	2.20	0.41
1:A:164:LEU:O	1:A:168:ILE:HG12	2.20	0.41
2:B:93:LYS:HE3	2:B:93:LYS:HB2	1.78	0.41
2:B:33:VAL:HA	2:B:36:GLU:CG	2.51	0.40
2:B:38:ALA:HB1	2:B:48:SER:O	2.21	0.40
2:B:39:HIS:CE1	2:B:45:HIS:HB2	2.57	0.40
1:C:224:GLN:O	1:C:261:ARG:HD3	2.21	0.40
1:C:401:HIS:CE1	1:C:403:GLU:HG2	2.56	0.40
1:A:209:LEU:HD12	1:A:209:LEU:HA	1.81	0.40
2:B:59:LEU:HD21	2:B:124:VAL:HA	2.03	0.40
2:B:164:THR:O	2:B:199:VAL:N	2.40	0.40
2:D:241:SER:C	2:D:243:THR:N	2.79	0.40
1:A:396:ILE:HG12	1:A:408:LEU:HD21	2.04	0.40
2:B:244:PHE:HB2	2:B:258:ASP:OD1	2.20	0.40
1:C:389:GLN:HA	1:C:392:LEU:HD12	2.02	0.40
2:D:282:HIS:CB	2:D:308:ARG:HB2	2.51	0.40
2:D:311:ALA:O	2:D:312:LYS:C	2.63	0.40
2:B:183:VAL:HB	2:B:187:SER:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:PHE:CE2	1:C:189:VAL:HG23	2.57	0.40
1:C:199:GLN:HE21	1:C:199:GLN:HB3	1.72	0.40
2:D:133:ASP:O	2:D:173: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	249/384 (65%)	236 (95%)	13 (5%)	0	100	100
1	C	246/384 (64%)	234 (95%)	12 (5%)	0	100	100
2	B	287/360 (80%)	275 (96%)	12 (4%)	0	100	100
2	D	278/360 (77%)	267 (96%)	11 (4%)	0	100	100
All	All	1060/1488 (71%)	1012 (96%)	48 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	242/347 (70%)	232 (96%)	10 (4%)	27	36
1	C	239/347 (69%)	232 (97%)	7 (3%)	37	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	273/329 (83%)	265 (97%)	8 (3%)	37	49
2	D	267/329 (81%)	266 (100%)	1 (0%)	84	91
All	All	1021/1352 (76%)	995 (98%)	26 (2%)	42	55

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	GLU
1	A	104	LYS
1	A	161	ASP
1	A	164	LEU
1	A	165	LYS
1	A	166	HIS
1	A	185	ARG
1	A	208	THR
1	A	369	ILE
1	A	418	LEU
2	B	30	GLU
2	B	45	HIS
2	B	92	LEU
2	B	95	LEU
2	B	109	ILE
2	B	261	ILE
2	B	275	ARG
2	B	312	LYS
1	C	98	GLU
1	C	165	LYS
1	C	204	TRP
1	C	208	THR
1	C	342	ARG
1	C	369	ILE
1	C	434	ARG
2	D	176	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	A	447	GLN
2	B	313	HIS

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Mol	Chain	Res	Type
1	C	367	HIS
1	C	387	GLN
1	C	447	GLN
2	D	198	GLN
2	D	333	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	261/384 (67%)	-0.95	0 100 100	44, 64, 94, 107	0
1	C	258/384 (67%)	-0.97	0 100 100	38, 64, 93, 116	0
2	B	295/360 (81%)	-0.95	0 100 100	37, 59, 94, 108	0
2	D	288/360 (80%)	-0.96	0 100 100	36, 58, 88, 104	0
All	All	1102/1488 (74%)	-0.96	0 100 100	36, 61, 93, 116	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.