



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:30 PM UTC

PDB ID : 5XTY / pdb_00005xty
Title : Crystal Structure of 11S allergen from Cocos nucifera L.
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Deposited on : 2017-06-21
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

<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

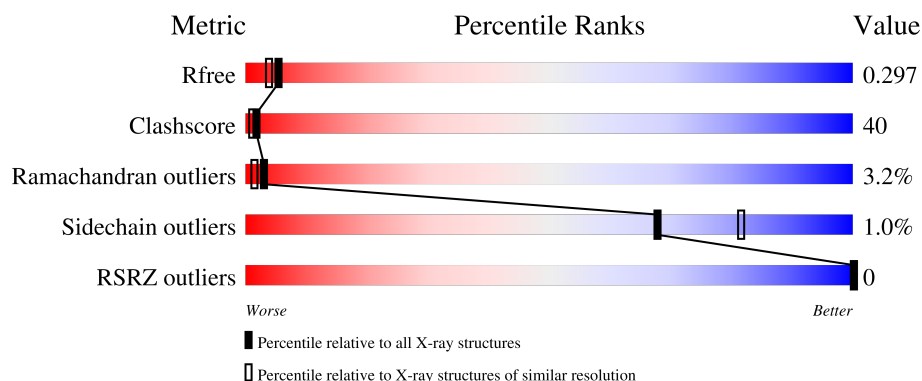
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

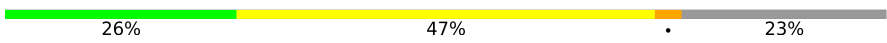
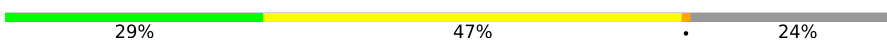
The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	466	
1	B	466	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5768 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 11S globulin isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2812	1745	522	526	19			
1	B	356	Total	C	N	O	S	0	0	0
			2800	1740	524	519	17			

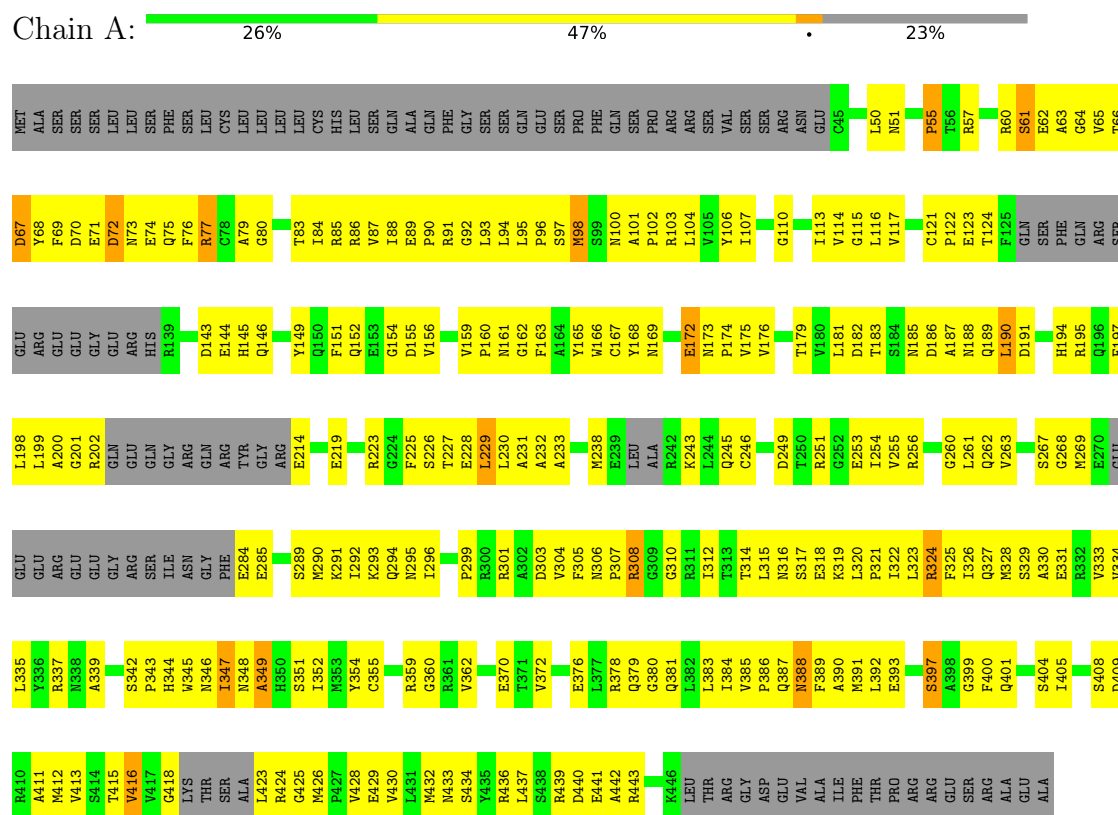
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	70	Total	O	0	0
			70	70		
2	B	86	Total	O	0	0
			86	86		

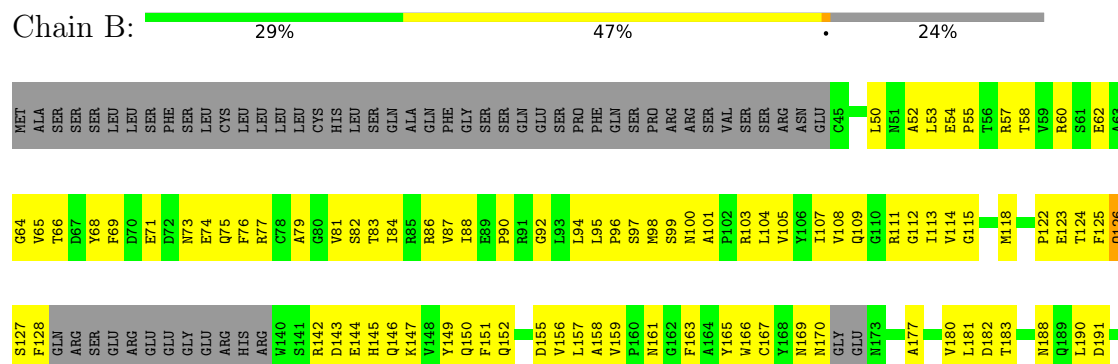
3 Residue-property plots

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: 11S globulin isoform 1



• Molecule 1: 11S globulin isoform 1



ARG	GLU	SER	ARG	ALA	GLU	ALA
M328	S329	A330	E331	V334	L335	Y336
						R337
						N338
						A339
						M340
						V341
						S342
						P343
						H344
						W345
						N346
						I347
						N348
						S351
						I352
						M353
						Y354
						C355
						T356
						R359
						G360
						R361
						V362
						E363
						V364
						A365
						D366
						D367
						F373
						D374
						G375
						E376
						L377
						R378
						Q379
						L382
						L383
						I384
						V385
						P386
						Q387
						N388
						F389
						A390
						M391
						L392
						E393
						R394
						A395
						R444
						V445
						K446
						L447
						T448
						ARG
						GLY
						ASP
						GLU
						VAL
						ALA
						ILE
						PHE
						THR
						PRO
						ARG
R195	Q196	F197	L198		G201	E202
						GLN
						GLU
						GLN
						GLY
						ARG
						GLN
						ARG
						TYR
						GLY
						ARG
						ILE
						GLU
						GLY
						SER
						ILE
						LYS
						E219
						N220
						I221
						L222
						R223
						T227
						E228
						L229
						L230
						A231
						A232
						A233
						F234
						G235
						V236
						N237
						M238
						E239
						L240
						A241
						R242
						Q245
						C246
						R247
						D248
						D249
						T250
						R251
						G252
						E253
						I254
						V255
						R256
						A257
						G260
						L264
						R265
						P266
						S267
						GLY
						MET
						GLU
						GLU
						GLU
						GLY
						ARG
						ILE
						ASN
						G282
						F283
						E284
						E285
						T286
						Y287
						C288
						S289
						M290
						K291
						I292
						K293
						Q294
						N295
						D298
						R301
						A302
						D303
						N306
						P307
						R308
						G309
						I312
						T313
						T314
						L315
						E318
						K319
						L320
						P321
						I322
						L323
						R324
						F325
						I326
						Q327

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	92.06Å 92.06Å 212.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.83 – 2.20 29.83 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.83-2.20) 99.7 (29.83-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	22.14 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.199 , 0.299 0.200 , 0.297	Depositor DCC
R_{free} test set	1708 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 125.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.398 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.530 for k,h,-l	Depositor
Outliers	0 of 33978 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5768	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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	0.50	0/2853	0.64	0/3845
1	B	0.50	0/2843	0.63	0/3833
All	All	0.50	0/5696	0.64	0/7678

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	349	ALA	Peptide

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	2812	0	2772	239	3
1	B	2800	0	2765	222	3
2	A	70	0	0	36	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	86	0	0	25	1
All	All	5768	0	5537	447	6

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 40.

All (447) 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:B:100:ASN:O	1:B:161:ASN:ND2	1.98	0.96
1:B:88:ILE:O	1:B:169:ASN:ND2	1.96	0.96
1:A:323:LEU:O	1:A:409:ASP:OD2	1.83	0.95
1:B:238:MET:SD	1:B:238:MET:N	2.37	0.93
1:A:318:GLU:HB3	1:B:290:MET:HB3	1.52	0.91
1:B:291:LYS:NZ	1:B:293:LYS:O	2.05	0.89
1:A:291:LYS:NZ	1:A:293:LYS:O	2.05	0.88
1:A:238:MET:SD	1:A:238:MET:N	2.46	0.87
1:B:424:ARG:NH1	2:B:503:HOH:O	2.07	0.87
1:B:111:ARG:HA	1:B:152:GLN:HA	1.55	0.86
1:B:291:LYS:HG2	2:B:506:HOH:O	1.75	0.86
1:A:429:GLU:O	1:A:433:ASN:ND2	2.09	0.86
1:A:296:ILE:HD12	1:A:315:LEU:HB2	1.58	0.85
1:B:81:VAL:HG12	1:B:182:ASP:HA	1.59	0.85
1:A:227:THR:O	1:A:231:ALA:N	2.10	0.84
1:A:413:VAL:O	1:B:282:GLY:N	2.12	0.82
1:B:293:LYS:N	2:B:506:HOH:O	2.10	0.82
1:A:384:ILE:O	2:A:501:HOH:O	1.98	0.82
1:A:100:ASN:O	1:A:161:ASN:ND2	2.12	0.81
1:B:351:SER:HB2	1:B:385:VAL:HG13	1.62	0.81
1:A:251:ARG:HB2	1:A:255:VAL:HG12	1.62	0.81
1:A:439:ARG:HH12	1:A:443:ARG:HB2	1.46	0.81
1:B:180:VAL:HG21	1:B:405:ILE:HG21	1.62	0.80
1:B:430:VAL:O	1:B:434:SER:OG	2.00	0.80
1:A:436:ARG:O	2:A:502:HOH:O	1.99	0.80
1:B:342:SER:O	1:B:344:HIS:ND1	2.13	0.79
1:A:229:LEU:O	1:A:233:ALA:N	2.15	0.79
1:A:183:THR:O	1:A:188:ASN:ND2	2.15	0.78
1:B:66:THR:HG23	1:B:86:ARG:HG3	1.65	0.77
1:A:191:ASP:OD1	1:A:195:ARG:NH2	2.15	0.77
1:B:60:ARG:HA	1:B:65:VAL:HG23	1.68	0.76
1:A:106:TYR:CE1	1:A:156:VAL:HG22	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLY:O	2:A:503:HOH:O	2.04	0.76
1:A:379:GLN:NE2	2:A:516:HOH:O	2.20	0.75
1:A:152:GLN:N	1:A:155:ASP:OD2	2.19	0.74
1:A:347:ILE:HD12	1:A:412:MET:HE3	1.68	0.74
1:B:282:GLY:O	2:B:502:HOH:O	2.05	0.74
1:B:52:ALA:O	2:B:501:HOH:O	2.04	0.74
1:B:219:GLU:N	2:B:511:HOH:O	2.20	0.74
1:A:186:ASP:OD2	2:A:504:HOH:O	2.06	0.74
1:B:245:GLN:N	1:B:245:GLN:OE1	2.21	0.73
1:B:318:GLU:OE1	1:B:410:ARG:NH1	2.22	0.73
1:B:245:GLN:HB2	1:B:247:ARG:HE	1.54	0.73
1:B:100:ASN:HB2	1:B:195:ARG:H	1.54	0.73
1:B:79:ALA:O	2:B:504:HOH:O	2.07	0.72
1:A:87:VAL:HG13	1:A:176:VAL:HG22	1.71	0.72
1:B:183:THR:O	1:B:188:ASN:ND2	2.21	0.72
1:A:415:THR:O	1:A:418:GLY:N	2.23	0.72
1:A:428:VAL:HG22	1:A:432:MET:HE2	1.70	0.72
1:B:57:ARG:NH1	2:B:513:HOH:O	2.23	0.72
1:A:228:GLU:OE2	1:A:228:GLU:N	2.15	0.72
1:A:194:HIS:O	2:A:505:HOH:O	2.07	0.71
1:A:291:LYS:O	1:A:322:ILE:HD11	1.90	0.71
1:A:348:ASN:OD1	1:A:412:MET:N	2.22	0.71
1:B:105:VAL:O	1:B:157:LEU:N	2.21	0.71
1:A:63:ALA:HB3	1:A:254:ILE:HG22	1.71	0.71
1:B:53:LEU:HD12	1:B:382:LEU:HD22	1.72	0.71
1:B:293:LYS:O	2:B:506:HOH:O	2.08	0.71
1:A:172:GLU:OE1	1:A:173:ASN:ND2	2.23	0.70
1:A:113:ILE:O	2:A:506:HOH:O	2.08	0.70
1:A:387:GLN:O	1:A:389:PHE:N	2.23	0.70
1:B:74:GLU:OE2	1:B:77:ARG:NH2	2.23	0.70
1:A:87:VAL:HG22	1:A:176:VAL:HG13	1.74	0.69
1:B:58:THR:O	2:B:507:HOH:O	2.09	0.69
1:A:290:MET:HA	1:B:318:GLU:HB3	1.75	0.69
1:A:284:GLU:HG2	1:A:285:GLU:HG2	1.73	0.69
1:A:103:ARG:HB2	1:A:159:VAL:HB	1.74	0.69
1:B:314:THR:O	1:B:319:LYS:NZ	2.17	0.69
1:A:115:GLY:HA3	1:A:166:TRP:CZ2	2.27	0.69
1:A:202:ARG:NH1	1:A:219:GLU:OE2	2.26	0.69
1:B:249:ASP:OD2	1:B:251:ARG:NH2	2.27	0.67
1:A:345:TRP:CD1	1:A:388:ASN:HA	2.30	0.67
1:A:70:ASP:HB3	1:A:73:ASN:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ILE:HA	1:A:322:ILE:HD11	1.77	0.67
1:A:327:GLN:HG2	1:A:409:ASP:OD1	1.94	0.67
1:B:95:LEU:N	1:B:253:GLU:O	2.21	0.67
1:A:117:VAL:HG12	1:A:146:GLN:HB2	1.76	0.67
1:A:144:GLU:O	2:A:507:HOH:O	2.12	0.66
1:B:331:GLU:HB3	1:B:404:SER:HB3	1.76	0.66
1:A:115:GLY:HA3	1:A:166:TRP:CE2	2.31	0.66
1:A:381:GLN:NE2	2:A:522:HOH:O	2.27	0.66
1:A:317:SER:O	2:A:508:HOH:O	2.13	0.66
1:B:236:VAL:HG22	1:B:237:ASN:H	1.62	0.65
1:A:110:GLY:HA3	1:A:175:VAL:HG22	1.76	0.65
1:B:412:MET:O	2:B:508:HOH:O	2.13	0.65
1:A:91:ARG:NH1	1:A:168:TYR:OH	2.29	0.65
1:A:55:PRO:O	2:A:509:HOH:O	2.13	0.65
1:B:359:ARG:N	1:B:399:GLY:O	2.30	0.65
1:A:360:GLY:HA3	1:A:400:PHE:CD2	2.32	0.65
1:B:98:MET:HG3	1:B:197:PHE:HB2	1.78	0.65
1:B:54:GLU:O	2:B:509:HOH:O	2.15	0.64
1:B:111:ARG:NH1	2:B:518:HOH:O	2.29	0.64
1:A:349:ALA:HB2	1:A:411:ALA:HB1	1.80	0.64
1:A:225:PHE:O	2:A:510:HOH:O	2.15	0.64
1:A:331:GLU:N	1:A:404:SER:O	2.22	0.63
1:A:228:GLU:O	1:A:232:ALA:N	2.20	0.63
1:A:303:ASP:N	1:A:312:ILE:O	2.30	0.63
1:B:101:ALA:HB3	1:B:181:LEU:HB3	1.79	0.63
1:B:122:PRO:HD2	1:B:284:GLU:HG2	1.80	0.63
1:B:303:ASP:OD2	1:B:314:THR:N	2.28	0.63
1:A:66:THR:HG23	1:A:86:ARG:HG2	1.81	0.62
1:B:109:GLN:NE2	2:B:519:HOH:O	2.29	0.62
1:A:62:GLU:OE1	2:A:511:HOH:O	2.16	0.62
1:A:312:ILE:HG12	1:A:333:VAL:HG22	1.82	0.62
1:B:334:VAL:HG13	1:B:401:GLN:HG3	1.82	0.62
1:A:61:SER:OG	1:A:254:ILE:HD12	1.99	0.61
1:A:72:ASP:HB2	1:A:77:ARG:NH2	2.15	0.61
1:B:115:GLY:HA3	1:B:166:TRP:CZ2	2.35	0.61
1:A:182:ASP:OD2	1:A:185:ASN:ND2	2.27	0.61
1:B:231:ALA:O	1:B:235:GLY:N	2.31	0.61
1:B:361:ARG:HD3	1:B:374:ASP:OD1	2.01	0.61
1:A:114:VAL:N	1:A:149:TYR:O	2.27	0.61
1:B:315:LEU:HB3	1:B:330:ALA:HB3	1.82	0.61
1:B:143:ASP:OD1	1:B:144:GLU:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:GLN:CB	1:B:247:ARG:HE	2.14	0.60
1:A:256:ARG:N	2:A:511:HOH:O	2.34	0.60
1:B:303:ASP:N	1:B:312:ILE:O	2.32	0.60
1:B:247:ARG:HG2	1:B:248:ASP:H	1.67	0.60
1:A:107:ILE:O	1:A:154:GLY:N	2.33	0.60
1:B:364:VAL:HB	1:B:373:PHE:HB3	1.84	0.60
1:A:346:ASN:HB3	1:A:349:ALA:HB3	1.83	0.59
1:A:416:VAL:HG13	1:A:423:LEU:HG	1.84	0.59
1:A:359:ARG:NH1	2:A:523:HOH:O	2.34	0.59
1:B:286:THR:OG1	1:B:287:TYR:N	2.31	0.59
1:B:247:ARG:H	1:B:247:ARG:HD2	1.67	0.59
1:A:387:GLN:C	1:A:389:PHE:H	2.08	0.59
1:A:95:LEU:N	1:A:253:GLU:O	2.34	0.59
1:A:116:LEU:HD11	1:A:163:PHE:HD2	1.68	0.59
1:B:74:GLU:HA	1:B:77:ARG:HB2	1.84	0.59
1:B:53:LEU:HB2	1:B:382:LEU:HB3	1.85	0.59
1:B:122:PRO:CD	1:B:284:GLU:HG2	2.33	0.59
1:A:106:TYR:HD2	1:A:405:ILE:HD11	1.68	0.59
1:A:439:ARG:HH22	1:A:443:ARG:HB3	1.67	0.59
1:A:249:ASP:OD1	1:A:251:ARG:NE	2.27	0.58
1:A:345:TRP:HD1	1:A:388:ASN:HA	1.68	0.58
1:A:351:SER:OG	1:A:385:VAL:HB	2.02	0.58
1:A:327:GLN:OE1	2:A:512:HOH:O	2.17	0.58
1:A:351:SER:OG	1:A:385:VAL:O	2.15	0.58
1:B:118:MET:HE3	1:B:292:ILE:HD11	1.85	0.58
1:A:91:ARG:NE	1:A:260:GLY:HA2	2.19	0.58
1:B:165:TYR:HD1	1:B:165:TYR:H	1.49	0.58
1:A:60:ARG:HA	1:A:65:VAL:HA	1.84	0.58
1:A:86:ARG:NH2	1:A:165:TYR:OH	2.31	0.58
1:A:343:PRO:HG3	1:A:392:LEU:HD21	1.86	0.58
1:A:344:HIS:N	2:A:524:HOH:O	2.36	0.57
1:A:94:LEU:HB3	1:A:167:CYS:HB2	1.86	0.57
1:B:353:MET:HG2	1:B:385:VAL:HG12	1.86	0.57
1:B:324:ARG:O	1:B:324:ARG:NH1	2.36	0.57
1:A:378:ARG:NH2	2:A:523:HOH:O	2.32	0.57
1:B:327:GLN:HA	1:B:409:ASP:OD1	2.04	0.57
1:B:108:VAL:H	1:B:177:ALA:HA	1.70	0.57
1:B:113:ILE:HA	1:B:150:GLN:HA	1.87	0.57
1:A:354:TYR:OH	1:A:380:GLY:HA2	2.05	0.57
1:A:245:GLN:OE1	1:A:245:GLN:N	2.34	0.57
1:A:103:ARG:N	1:A:159:VAL:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:O	2:A:513:HOH:O	2.18	0.56
1:A:360:GLY:N	1:A:376:GLU:OE2	2.37	0.56
1:A:437:LEU:HB2	2:A:548:HOH:O	2.03	0.56
1:B:83:THR:HB	1:B:180:VAL:HG12	1.88	0.56
1:A:95:LEU:HG	1:A:253:GLU:HA	1.88	0.56
1:A:262:GLN:NE2	1:A:263:VAL:O	2.39	0.56
1:A:342:SER:O	1:A:344:HIS:ND1	2.27	0.56
1:B:249:ASP:CG	1:B:251:ARG:HH21	2.14	0.56
1:B:353:MET:HE3	1:B:402:LEU:HD12	1.87	0.56
1:B:94:LEU:HA	1:B:254:ILE:HA	1.88	0.55
1:B:241:ALA:O	1:B:245:GLN:OE1	2.24	0.55
1:A:91:ARG:HE	1:A:260:GLY:HA2	1.72	0.55
1:B:346:ASN:OD1	1:B:351:SER:OG	2.22	0.55
1:A:98:MET:HE3	1:A:162:GLY:HA2	1.88	0.55
1:B:306:ASN:O	1:B:309:GLY:HA2	2.07	0.55
1:A:101:ALA:HB3	1:A:181:LEU:HB3	1.89	0.55
1:A:223:ARG:HD3	1:A:245:GLN:HB3	1.89	0.54
1:A:83:THR:OG1	1:A:179:THR:O	2.12	0.54
1:A:439:ARG:HH22	1:A:443:ARG:HD2	1.72	0.54
1:A:352:ILE:HG13	1:A:384:ILE:HD13	1.90	0.54
1:A:107:ILE:HG21	1:A:151:PHE:CD2	2.43	0.54
1:A:423:LEU:O	1:A:425:GLY:N	2.40	0.54
1:B:356:THR:O	2:B:510:HOH:O	2.18	0.54
1:B:351:SER:N	1:B:385:VAL:O	2.36	0.54
1:A:106:TYR:CD2	1:A:405:ILE:HD11	2.42	0.54
1:A:166:TRP:HD1	2:A:560:HOH:O	1.90	0.54
1:B:231:ALA:HB1	1:B:236:VAL:O	2.08	0.53
1:B:361:ARG:HA	1:B:376:GLU:HA	1.90	0.53
1:A:181:LEU:HD13	1:A:194:HIS:CD2	2.44	0.53
1:A:195:ARG:HA	2:A:505:HOH:O	2.08	0.53
1:A:124:THR:OG1	2:A:515:HOH:O	2.18	0.53
1:B:142:ARG:NH2	2:B:526:HOH:O	2.40	0.53
1:A:107:ILE:HG21	1:A:151:PHE:HD2	1.73	0.53
1:B:291:LYS:NZ	2:B:506:HOH:O	2.41	0.53
1:A:423:LEU:C	1:A:425:GLY:H	2.16	0.53
1:B:105:VAL:HB	1:B:157:LEU:HB2	1.91	0.53
1:A:198:LEU:HD12	1:A:200:ALA:O	2.08	0.53
1:B:99:SER:OG	1:B:103:ARG:NH1	2.42	0.53
1:B:158:ALA:HB1	1:B:326:ILE:HD12	1.91	0.53
1:A:327:GLN:HA	1:A:409:ASP:CG	2.34	0.52
1:A:384:ILE:HG22	2:A:518:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ILE:HD12	1:B:155:ASP:HB2	1.91	0.52
1:A:355:CYS:SG	1:A:379:GLN:HA	2.50	0.52
1:A:284:GLU:HB3	1:B:412:MET:HG2	1.91	0.52
1:B:152:GLN:NE2	1:B:155:ASP:OD1	2.43	0.52
1:B:395:ALA:HB2	1:B:400:PHE:HB2	1.91	0.52
1:B:103:ARG:HE	1:B:159:VAL:HB	1.74	0.52
1:B:298:ASP:O	1:B:301:ARG:N	2.40	0.52
1:A:301:ARG:O	1:B:147:LYS:NZ	2.34	0.52
1:B:114:VAL:HG23	1:B:167:CYS:HB3	1.91	0.52
1:B:237:ASN:OD1	1:B:240:LEU:N	2.35	0.52
1:A:92:GLY:HA2	1:A:256:ARG:HG3	1.92	0.52
1:A:318:GLU:C	1:B:321:PRO:HG2	2.35	0.52
1:B:88:ILE:HG12	1:B:254:ILE:HG21	1.91	0.51
1:B:284:GLU:HB3	1:B:288:CYS:HB2	1.92	0.51
1:B:353:MET:N	1:B:383:LEU:O	2.42	0.51
1:B:90:PRO:HA	1:B:169:ASN:CG	2.35	0.51
1:A:334:VAL:HG13	1:A:401:GLN:HG2	1.92	0.51
1:B:127:SER:HB2	1:B:264:LEU:CD2	2.40	0.51
1:B:308:ARG:N	1:B:309:GLY:HA2	2.26	0.51
1:A:346:ASN:HA	1:A:413:VAL:HG12	1.93	0.51
1:B:309:GLY:HA3	1:B:336:TYR:CD2	2.45	0.51
1:B:327:GLN:HA	1:B:409:ASP:CG	2.35	0.51
1:B:344:HIS:NE2	1:B:391:MET:HE3	2.25	0.51
1:B:438:SER:OG	1:B:439:ARG:N	2.43	0.50
1:A:376:GLU:HG2	1:A:378:ARG:NH1	2.26	0.50
1:B:201:GLY:O	1:B:220:ASN:HB3	2.11	0.50
1:A:77:ARG:O	1:A:80:GLY:N	2.41	0.50
1:A:114:VAL:HG12	2:A:538:HOH:O	2.11	0.50
1:B:424:ARG:HG2	2:B:568:HOH:O	2.10	0.50
1:B:103:ARG:HG2	1:B:159:VAL:HB	1.94	0.50
1:B:427:PRO:HD2	1:B:430:VAL:HG21	1.93	0.50
1:A:61:SER:N	1:A:64:GLY:O	2.36	0.50
1:B:96:PRO:HA	1:B:165:TYR:O	2.12	0.50
1:B:191:ASP:N	1:B:191:ASP:OD1	2.42	0.50
1:B:359:ARG:HD2	2:B:574:HOH:O	2.12	0.50
1:A:189:GLN:O	1:A:190:LEU:HB2	2.11	0.50
1:A:314:THR:O	1:A:319:LYS:HD2	2.12	0.50
1:A:57:ARG:HB2	1:A:68:TYR:HB2	1.93	0.50
1:B:444:ARG:O	1:B:448:THR:HG23	2.12	0.50
1:A:64:GLY:HA3	1:A:87:VAL:O	2.12	0.49
1:A:72:ASP:HB2	1:A:77:ARG:HH21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:PHE:CD2	1:B:83:THR:HG23	2.47	0.49
1:B:115:GLY:N	1:B:166:TRP:O	2.34	0.49
1:A:370:GLU:OE1	2:A:514:HOH:O	2.18	0.49
1:A:429:GLU:HA	1:A:432:MET:HE3	1.94	0.49
1:A:123:GLU:HB3	1:A:145:HIS:C	2.37	0.49
1:A:331:GLU:HB2	1:A:404:SER:HB3	1.94	0.49
1:B:126:GLN:HA	1:B:144:GLU:HG2	1.95	0.49
1:A:415:THR:HG23	1:A:418:GLY:HA3	1.95	0.49
1:B:341:VAL:HG12	1:B:393:GLU:HG2	1.93	0.49
1:B:64:GLY:HA3	1:B:87:VAL:O	2.12	0.49
1:B:124:THR:C	1:B:125:PHE:HD1	2.20	0.49
1:B:377:LEU:HB2	1:B:400:PHE:HZ	1.77	0.49
1:A:121:CYS:HB3	2:A:550:HOH:O	2.12	0.49
1:A:343:PRO:HA	1:A:391:MET:O	2.13	0.49
1:A:415:THR:O	1:A:416:VAL:C	2.56	0.49
1:B:341:VAL:HG13	1:B:344:HIS:HE1	1.78	0.49
1:A:96:PRO:HB2	1:A:199:LEU:HB2	1.94	0.48
1:B:157:LEU:HD23	1:B:293:LYS:HB3	1.94	0.48
1:B:289:SER:O	1:B:289:SER:OG	2.31	0.48
1:A:71:GLU:C	1:A:73:ASN:H	2.20	0.48
1:B:415:THR:CG2	1:B:421:SER:HB3	2.43	0.48
1:A:95:LEU:HD22	1:A:200:ALA:HB3	1.96	0.48
1:A:98:MET:HE2	1:A:197:PHE:HB2	1.96	0.48
1:B:359:ARG:HH12	1:B:398:ALA:CB	2.26	0.48
1:B:228:GLU:OE1	1:B:228:GLU:N	2.36	0.48
1:A:67:ASP:N	1:A:85:ARG:O	2.37	0.48
1:B:69:PHE:HB2	1:B:83:THR:O	2.14	0.48
1:B:247:ARG:NH1	2:B:527:HOH:O	2.41	0.48
1:B:242:ARG:HG3	1:B:247:ARG:HD3	1.94	0.48
1:A:289:SER:O	1:A:289:SER:OG	2.32	0.47
1:B:114:VAL:HB	1:B:151:PHE:CD2	2.49	0.47
1:A:318:GLU:HB3	1:B:290:MET:CB	2.36	0.47
1:A:344:HIS:O	1:A:391:MET:N	2.44	0.47
1:B:292:ILE:N	2:B:506:HOH:O	2.47	0.47
1:A:91:ARG:HB2	1:A:256:ARG:HG2	1.95	0.47
1:A:386:PRO:HG2	1:A:389:PHE:CD2	2.50	0.47
1:B:323:LEU:HD23	1:B:323:LEU:HA	1.74	0.47
1:A:95:LEU:HD12	1:A:253:GLU:HA	1.96	0.47
1:A:100:ASN:ND2	2:A:529:HOH:O	2.48	0.47
1:B:107:ILE:HD11	1:B:157:LEU:HD21	1.95	0.47
1:B:339:ALA:O	1:B:394:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:ARG:HH22	1:A:443:ARG:CB	2.27	0.47
1:B:361:ARG:HG3	1:B:362:VAL:N	2.29	0.47
1:A:223:ARG:CD	1:A:245:GLN:HB3	2.45	0.46
1:B:71:GLU:HG2	1:B:82:SER:OG	2.15	0.46
1:B:125:PHE:CE2	1:B:147:LYS:HA	2.49	0.46
1:B:423:LEU:C	1:B:425:GLY:H	2.22	0.46
1:B:145:HIS:ND1	1:B:146:GLN:O	2.40	0.46
1:B:115:GLY:HA3	1:B:166:TRP:CE2	2.49	0.46
1:B:161:ASN:O	1:B:163:PHE:HD1	1.99	0.46
1:B:242:ARG:O	1:B:245:GLN:N	2.47	0.46
1:B:322:ILE:HA	1:B:325:PHE:HD1	1.80	0.46
1:A:50:LEU:HD23	1:A:50:LEU:HA	1.56	0.46
1:A:428:VAL:O	1:A:432:MET:HG3	2.16	0.46
1:B:74:GLU:OE2	1:B:77:ARG:CZ	2.63	0.46
1:B:295:ASN:O	1:B:301:ARG:HD2	2.16	0.46
1:A:107:ILE:HG12	1:A:151:PHE:CD2	2.50	0.46
1:B:326:ILE:HG22	1:B:328:MET:HB2	1.97	0.46
1:A:75:GLN:NE2	2:A:528:HOH:O	2.46	0.46
1:A:95:LEU:CG	1:A:253:GLU:HA	2.45	0.46
1:A:299:PRO:C	1:A:301:ARG:H	2.23	0.46
1:A:440:ASP:OD1	1:A:441:GLU:N	2.49	0.46
1:B:322:ILE:HA	1:B:325:PHE:CD1	2.51	0.46
1:B:415:THR:HG23	1:B:421:SER:HB3	1.98	0.46
1:A:62:GLU:CD	1:A:251:ARG:HB3	2.41	0.46
1:A:102:PRO:HD2	1:A:182:ASP:O	2.15	0.46
1:A:143:ASP:HB3	1:A:144:GLU:H	1.55	0.46
1:B:245:GLN:HG2	1:B:247:ARG:HH21	1.81	0.46
1:A:326:ILE:HG22	1:A:328:MET:HG3	1.97	0.46
1:B:74:GLU:OE2	1:B:77:ARG:NE	2.48	0.46
1:B:432:MET:O	1:B:436:ARG:N	2.47	0.45
1:A:190:LEU:HB2	2:A:529:HOH:O	2.14	0.45
1:A:345:TRP:HB2	1:A:388:ASN:C	2.41	0.45
1:B:97:SER:HB3	1:B:198:LEU:HD23	1.97	0.45
1:B:391:MET:HG2	1:B:392:LEU:N	2.32	0.45
1:A:95:LEU:CD1	1:A:253:GLU:HA	2.47	0.45
1:A:439:ARG:NH1	1:A:443:ARG:HB2	2.23	0.45
1:B:76:PHE:CZ	1:B:83:THR:HG22	2.51	0.45
1:B:123:GLU:H	1:B:123:GLU:CD	2.24	0.45
1:B:125:PHE:CZ	1:B:147:LYS:HG3	2.52	0.45
1:B:236:VAL:HG22	1:B:237:ASN:ND2	2.31	0.45
1:A:61:SER:OG	1:A:253:GLU:OE2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ASN:HB2	1:A:195:ARG:HB2	1.97	0.45
1:B:424:ARG:HA	1:B:446:LYS:CG	2.47	0.45
1:A:349:ALA:O	1:A:387:GLN:HA	2.16	0.45
1:A:256:ARG:HB2	2:A:511:HOH:O	2.16	0.45
1:A:315:LEU:HB3	1:A:330:ALA:HB3	1.99	0.45
1:B:100:ASN:OD1	1:B:190:LEU:HD12	2.17	0.45
1:B:124:THR:O	1:B:125:PHE:HD1	2.00	0.45
1:A:93:LEU:O	1:A:254:ILE:HA	2.17	0.45
1:A:172:GLU:HB3	1:A:173:ASN:H	1.38	0.45
1:A:329:SER:HB2	1:A:408:SER:O	2.17	0.45
1:A:383:LEU:HD12	2:A:525:HOH:O	2.15	0.45
1:B:257:ALA:O	1:B:260:GLY:N	2.50	0.45
1:B:392:LEU:HD23	1:B:392:LEU:HA	1.71	0.45
1:B:355:CYS:SG	1:B:379:GLN:HA	2.56	0.45
1:A:437:LEU:HD13	1:A:441:GLU:HB3	1.99	0.45
1:A:344:HIS:O	1:A:390:ALA:HA	2.18	0.44
1:B:50:LEU:HB2	1:B:373:PHE:HB2	1.99	0.44
1:A:101:ALA:HB3	1:A:181:LEU:HD22	1.99	0.44
1:B:114:VAL:HG12	1:B:149:TYR:HB2	1.98	0.44
1:B:337:ARG:NH2	2:B:530:HOH:O	2.47	0.44
1:A:102:PRO:HD3	1:A:161:ASN:HD21	1.81	0.44
1:A:90:PRO:C	1:A:92:GLY:H	2.26	0.44
1:A:335:LEU:HA	1:A:335:LEU:HD23	1.67	0.44
1:A:362:VAL:HG22	1:A:393:GLU:HG2	1.98	0.44
1:B:105:VAL:HB	1:B:157:LEU:HD12	1.99	0.44
1:B:348:ASN:OD1	1:B:412:MET:N	2.47	0.44
1:A:432:MET:HB3	1:A:437:LEU:O	2.18	0.44
1:A:310:GLY:HA3	1:A:335:LEU:HD23	2.00	0.44
1:A:335:LEU:HD22	1:A:339:ALA:CB	2.48	0.44
1:A:73:ASN:HB3	1:A:76:PHE:HB2	2.00	0.44
1:B:62:GLU:OE2	1:B:256:ARG:HB2	2.17	0.44
1:B:387:GLN:O	1:B:389:PHE:N	2.49	0.44
1:A:324:ARG:C	1:A:409:ASP:OD2	2.60	0.43
1:B:437:LEU:HD13	1:B:441:GLU:HB2	2.00	0.43
1:A:430:VAL:O	1:A:434:SER:OG	2.35	0.43
1:B:68:TYR:CD2	1:B:84:ILE:HG13	2.53	0.43
1:B:223:ARG:HA	1:B:223:ARG:HD2	1.63	0.43
1:A:306:ASN:H	1:B:126:GLN:HG3	1.82	0.43
1:A:101:ALA:CB	1:A:181:LEU:HB3	2.49	0.43
1:A:226:SER:O	1:A:230:LEU:HB2	2.18	0.43
1:B:294:GLN:HB3	1:B:315:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ARG:HB2	1:A:397:SER:HA	2.01	0.43
1:A:397:SER:C	1:A:399:GLY:H	2.26	0.43
1:B:257:ALA:HB1	1:B:260:GLY:O	2.18	0.43
1:B:342:SER:HB2	1:B:415:THR:OG1	2.17	0.43
1:A:294:GLN:HE22	1:B:291:LYS:HE3	1.83	0.43
1:B:239:GLU:HB3	2:B:576:HOH:O	2.19	0.43
1:A:304:VAL:HG12	1:A:307:PRO:HD3	2.00	0.43
1:B:320:LEU:O	1:B:323:LEU:HB2	2.18	0.43
1:A:69:PHE:HB3	1:A:76:PHE:CE2	2.54	0.43
1:A:306:ASN:C	1:A:308:ARG:H	2.26	0.43
1:B:180:VAL:CG2	1:B:405:ILE:HD13	2.48	0.43
1:B:323:LEU:HD22	1:B:328:MET:O	2.19	0.43
1:A:51:ASN:HB3	2:A:541:HOH:O	2.19	0.42
1:A:317:SER:HA	1:A:320:LEU:O	2.19	0.42
1:A:359:ARG:HG3	1:A:376:GLU:OE2	2.19	0.42
1:A:251:ARG:CZ	1:A:255:VAL:HG11	2.49	0.42
1:A:423:LEU:C	1:A:425:GLY:N	2.74	0.42
1:B:73:ASN:OD1	1:B:75:GLN:HB2	2.19	0.42
1:B:351:SER:HB2	1:B:385:VAL:CG1	2.42	0.42
1:A:151:PHE:HE1	2:A:506:HOH:O	2.01	0.42
1:A:355:CYS:SG	1:A:400:PHE:HE1	2.42	0.42
1:B:88:ILE:HG22	1:B:169:ASN:HB2	2.01	0.42
1:B:404:SER:OG	1:B:406:LYS:HE3	2.19	0.42
1:A:88:ILE:HG22	1:A:89:GLU:O	2.20	0.42
1:A:89:GLU:C	1:A:169:ASN:HD22	2.27	0.42
1:A:97:SER:HB3	1:A:198:LEU:HD22	2.01	0.42
1:A:319:LYS:HE3	1:B:289:SER:OG	2.19	0.42
1:A:439:ARG:NH2	1:A:443:ARG:HD2	2.34	0.42
1:B:55:PRO:HG3	1:B:69:PHE:CE2	2.54	0.42
1:A:318:GLU:OE1	1:B:290:MET:HB3	2.19	0.42
1:B:395:ALA:CB	1:B:400:PHE:HB2	2.50	0.42
1:B:81:VAL:HA	1:B:183:THR:H	1.85	0.42
1:A:75:GLN:O	1:A:79:ALA:N	2.38	0.42
1:A:379:GLN:HG2	1:A:380:GLY:N	2.34	0.42
1:B:236:VAL:HG22	1:B:237:ASN:HD22	1.84	0.42
1:B:427:PRO:HB2	1:B:430:VAL:HG23	2.02	0.42
1:A:91:ARG:HH11	1:A:168:TYR:HH	1.64	0.41
1:A:187:ALA:O	1:A:189:GLN:N	2.52	0.41
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.80	0.41
1:B:90:PRO:C	1:B:92:GLY:H	2.29	0.41
1:B:387:GLN:C	1:B:389:PHE:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:PRO:O	1:A:124:THR:HG23	2.20	0.41
1:A:323:LEU:C	1:A:325:PHE:N	2.78	0.41
1:A:114:VAL:HG23	1:A:151:PHE:CD1	2.55	0.41
1:A:318:GLU:OE1	2:A:517:HOH:O	2.21	0.41
1:B:98:MET:HE3	1:B:197:PHE:CG	2.55	0.41
1:B:104:LEU:HD22	1:B:156:VAL:HG12	2.02	0.41
1:B:230:LEU:O	1:B:233:ALA:HB3	2.20	0.41
1:A:97:SER:CB	1:A:198:LEU:HD22	2.50	0.41
1:A:201:GLY:N	1:A:246:CYS:SG	2.84	0.41
1:A:316:ASN:C	1:A:323:LEU:HD12	2.45	0.41
1:B:242:ARG:HG3	1:B:247:ARG:CD	2.50	0.41
1:B:266:PRO:O	1:B:267:SER:OG	2.29	0.41
1:A:83:THR:OG1	1:A:84:ILE:N	2.48	0.41
1:A:294:GLN:NE2	1:B:291:LYS:HE3	2.35	0.41
1:A:294:GLN:OE1	1:A:295:ASN:N	2.53	0.41
1:B:128:PHE:HA	1:B:142:ARG:HG2	2.02	0.41
1:B:423:LEU:C	1:B:425:GLY:N	2.78	0.41
1:A:441:GLU:O	1:A:442:ALA:C	2.62	0.41
1:B:345:TRP:CD1	1:B:388:ASN:HA	2.56	0.41
1:B:359:ARG:HH12	1:B:398:ALA:HB3	1.84	0.41
1:B:360:GLY:O	1:B:377:LEU:N	2.33	0.41
1:B:435:TYR:HB2	1:B:437:LEU:HG	2.01	0.41
1:A:251:ARG:HB2	1:A:255:VAL:CG1	2.44	0.41
1:A:261:LEU:HD23	1:A:262:GLN:N	2.36	0.41
1:A:268:GLY:HA3	1:A:269:MET:HA	1.85	0.41
1:A:292:ILE:HA	1:A:322:ILE:CD1	2.49	0.41
1:A:391:MET:HE3	1:A:391:MET:HB2	1.78	0.41
1:B:228:GLU:HB2	2:B:525:HOH:O	2.21	0.41
1:B:407:THR:O	1:B:407:THR:OG1	2.33	0.41
1:B:107:ILE:CD1	1:B:155:ASP:HB2	2.51	0.41
1:B:221:ILE:HA	1:B:221:ILE:HD12	1.77	0.41
1:B:424:ARG:NH1	1:B:448:THR:O	2.54	0.41
1:B:112:GLY:HA3	1:B:151:PHE:CE1	2.56	0.40
1:B:320:LEU:HD12	1:B:320:LEU:HA	1.73	0.40
1:A:230:LEU:HD12	1:A:230:LEU:HA	1.81	0.40
1:A:321:PRO:HG3	1:B:321:PRO:HG3	2.03	0.40
1:B:284:GLU:HB3	1:B:288:CYS:CB	2.50	0.40
1:B:353:MET:HE1	1:B:404:SER:HB2	2.02	0.40
1:A:76:PHE:O	1:A:80:GLY:N	2.55	0.40
1:A:96:PRO:HB3	2:A:560:HOH:O	2.21	0.40
1:A:98:MET:CE	1:A:162:GLY:HA2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:PHE:O	1:B:125:PHE:HA	2.21	0.40
1:B:448:THR:O	2:B:503:HOH:O	2.22	0.40
1:A:83:THR:O	1:A:84:ILE:HG13	2.22	0.40
1:B:366:ASP:OD1	1:B:366:ASP:C	2.64	0.40
1:B:104:LEU:HA	1:B:157:LEU:O	2.21	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:504:HOH:O	2:B:562:HOH:O[3_545]	2.00	0.20
1:B:144:GLU:O	1:B:446:LYS:NZ[2_445]	2.12	0.08
1:A:426:MET:O	2:A:507:HOH:O[2_445]	2.13	0.07
1:A:243:LYS:NZ	1:A:441:GLU:OE2[3_545]	2.18	0.02
1:B:195:ARG:NH2	1:B:367:ASP:OD1[2_445]	2.18	0.02
1:A:214:GLU:O	1:B:227:THR:OG1[4_555]	2.19	0.01

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	347/466 (74%)	283 (82%)	46 (13%)	18 (5%)		
1	B	344/466 (74%)	298 (87%)	42 (12%)	4 (1%)		
All	All	691/932 (74%)	581 (84%)	88 (13%)	22 (3%)		

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	SER
1	B	266	PRO
1	A	61	SER

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Mol	Chain	Res	Type
1	A	347	ILE
1	A	388	ASN
1	A	416	VAL
1	A	424	ARG
1	B	374	ASP
1	A	72	ASP
1	A	77	ARG
1	A	172	GLU
1	A	308	ARG
1	B	236	VAL
1	A	74	GLU
1	A	160	PRO
1	A	190	LEU
1	A	229	LEU
1	A	324	ARG
1	A	174	PRO
1	A	55	PRO
1	A	372	VAL
1	B	386	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	299/399 (75%)	296 (99%)	3 (1%)	68	81
1	B	299/399 (75%)	296 (99%)	3 (1%)	68	81
All	All	598/798 (75%)	592 (99%)	6 (1%)	68	81

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ASP
1	A	98	MET
1	A	397	SER
1	B	126	GLN

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Mol	Chain	Res	Type
1	B	170	ASN
1	B	253	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	ASN
1	A	295	ASN
1	A	350	HIS
1	A	388	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	359/466 (77%)	-0.89	0 100 100	36, 52, 76, 149	0
1	B	356/466 (76%)	-0.94	0 100 100	35, 48, 67, 88	0
All	All	715/932 (76%)	-0.91	0 100 100	35, 50, 73, 149	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.