



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:15 PM UTC

PDB ID : 2QPA / pdb_00002qpa
Title : Crystal Structure of S.cerevisiae Vps4 in the presence of ADP
Authors : Xiao, J.; Xu, Z.
Deposited on : 2007-07-23
Resolution : 3.20 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

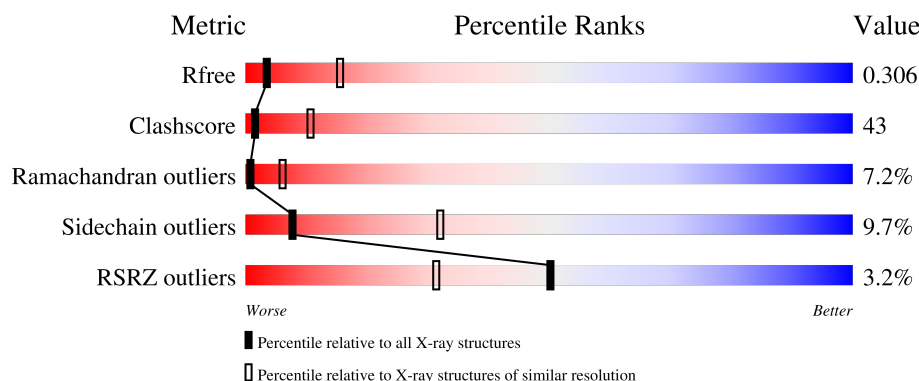
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	355	5% 35% 43% 8% 14%
1	B	355	3% 36% 42% 7% 15%
1	C	355	5% 32% 42% 9% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6415 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 Vacuolar protein sorting-associated protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2176	1388	364	418	6			
1	B	303	Total	C	N	O	S	0	0	0
			2120	1349	350	415	6			
1	C	296	Total	C	N	O	S	0	0	0
			2082	1327	342	407	6			

There are 9 discrepancies between the modelled and reference sequences:

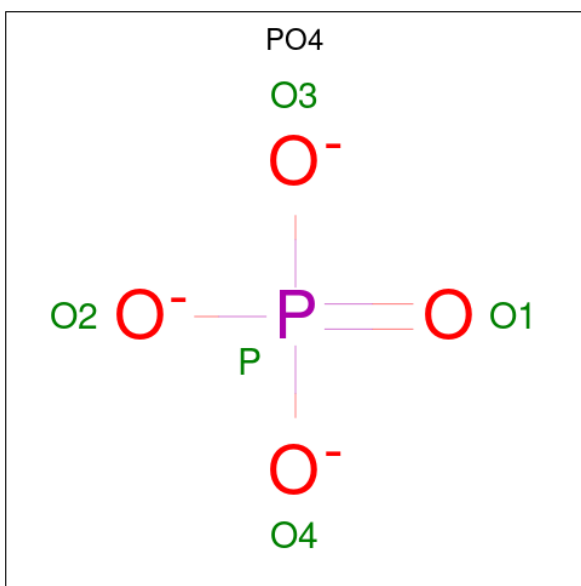
Chain	Residue	Modelled	Actual	Comment	Reference
A	233	GLN	GLU	engineered mutation	UNP P52917
A	317	SER	CYS	engineered mutation	UNP P52917
A	376	SER	CYS	engineered mutation	UNP P52917
B	233	GLN	GLU	engineered mutation	UNP P52917
B	317	SER	CYS	engineered mutation	UNP P52917
B	376	SER	CYS	engineered mutation	UNP P52917
C	233	GLN	GLU	engineered mutation	UNP P52917
C	317	SER	CYS	engineered mutation	UNP P52917
C	376	SER	CYS	engineered mutation	UNP P52917

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

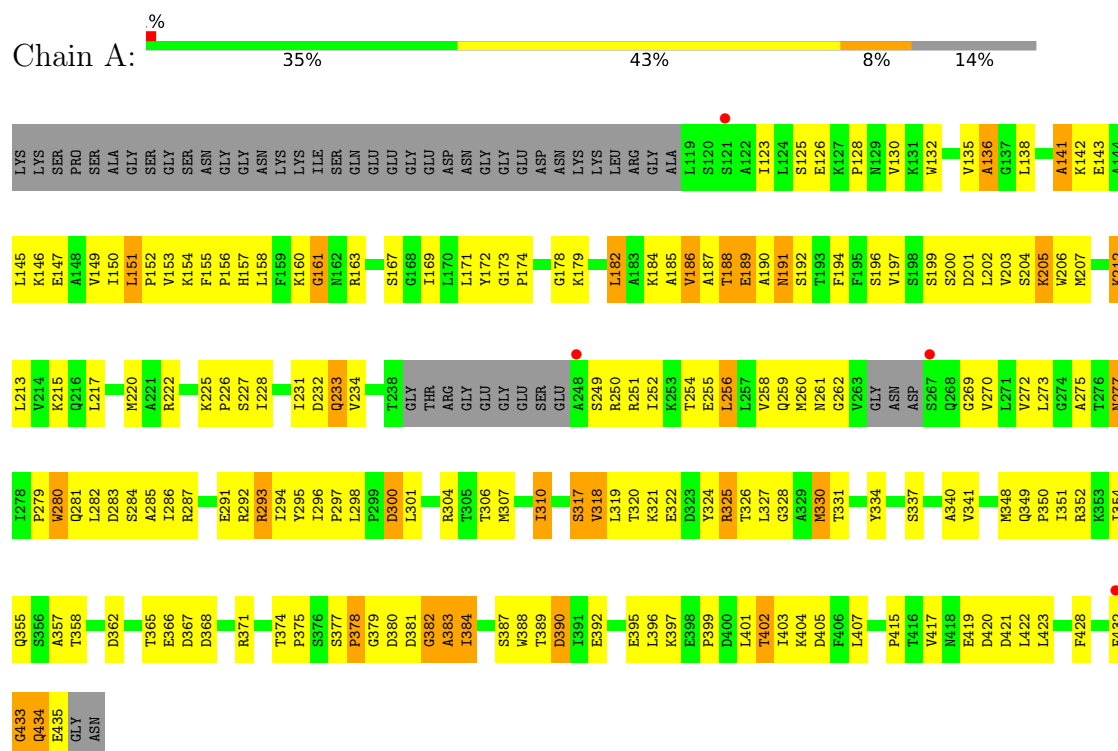


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 5	O 4	P 1	0	0
3	C	1	Total 5	O 4	P 1	0	0

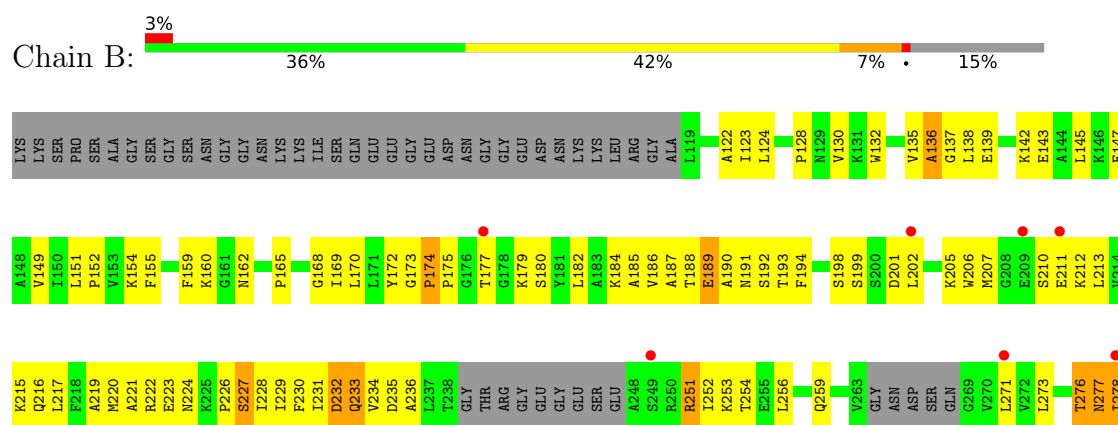
3 Residue-property plots

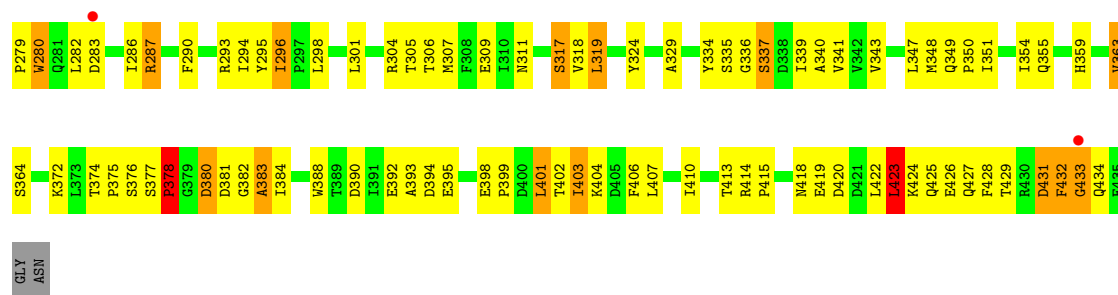
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Vacuolar protein sorting-associated protein 4

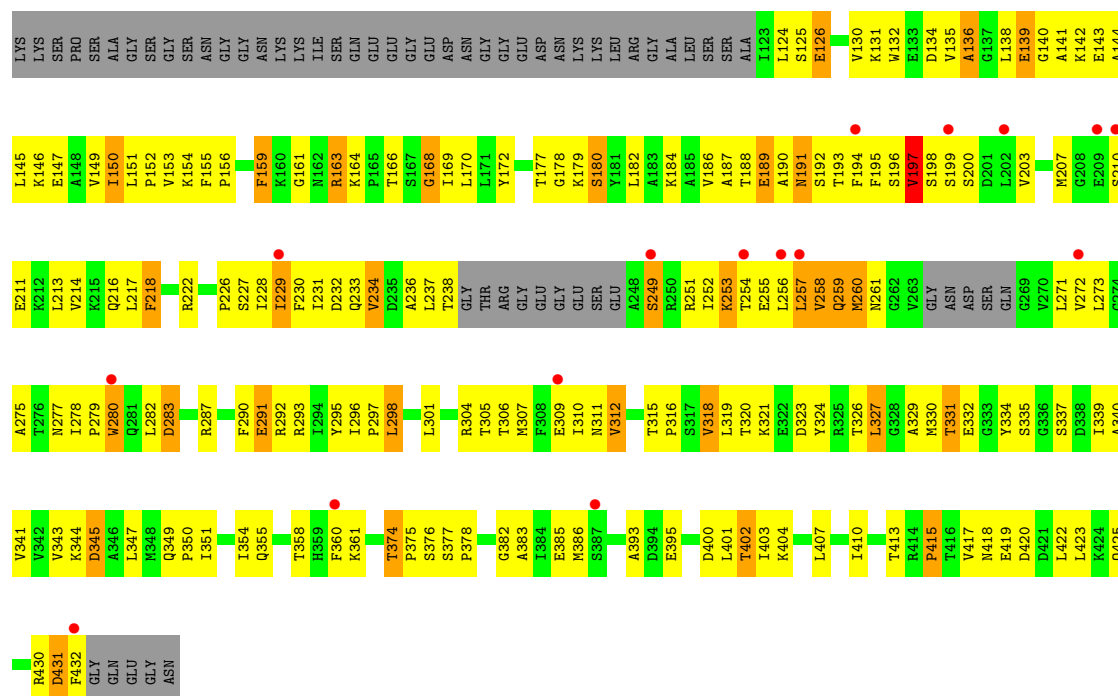


- Molecule 1: Vacuolar protein sorting-associated protein 4





• Molecule 1: Vacuolar protein sorting-associated protein 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.63Å 120.64Å 157.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 50.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.6 (50.00-3.20) 94.9 (50.00-3.20)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.255 , 0.305 0.257 , 0.306	Depositor DCC
R_{free} test set	1168 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	106.7	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 126.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6415	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, PO4

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	0.64	0/2215	1.07	16/3027 (0.5%)
1	B	0.55	0/2159	1.02	9/2959 (0.3%)
1	C	0.45	0/2121	0.93	6/2907 (0.2%)
All	All	0.55	0/6495	1.01	31/8893 (0.3%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	403	ILE	N-CA-C	-9.16	100.62	113.07
1	C	296	ILE	CA-C-N	8.94	128.79	120.21
1	C	296	ILE	C-N-CA	8.94	128.79	120.21
1	B	296	ILE	CA-C-N	6.72	126.69	120.03
1	B	296	ILE	C-N-CA	6.72	126.69	120.03
1	A	186	VAL	N-CA-C	-6.67	103.83	110.30
1	B	378	PRO	N-CA-CB	6.43	110.00	103.25
1	C	378	PRO	N-CA-CB	6.31	109.88	103.25
1	A	378	PRO	N-CA-CB	6.27	109.84	103.25
1	A	149	VAL	N-CA-C	6.21	116.52	111.62
1	A	296	ILE	CA-C-N	6.16	127.57	120.98
1	A	296	ILE	C-N-CA	6.16	127.57	120.98
1	A	277	ASN	N-CA-C	-5.92	105.36	113.30
1	A	250	ARG	N-CA-C	-5.90	106.16	113.19
1	C	179	LYS	N-CA-C	-5.90	105.58	112.89
1	A	135	VAL	N-CA-C	5.87	116.31	107.80
1	A	141	ALA	N-CA-C	-5.83	104.92	111.28
1	A	157	HIS	N-CA-C	5.77	117.65	111.36
1	B	227	SER	N-CA-C	5.71	115.64	108.45
1	B	174	PRO	CA-C-N	5.61	125.79	119.90
1	B	174	PRO	C-N-CA	5.61	125.79	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	425	GLN	N-CA-C	-5.45	105.42	111.36
1	A	293	ARG	N-CA-C	5.45	116.31	107.32
1	A	377	SER	N-CA-C	5.44	117.49	109.50
1	B	277	ASN	N-CA-C	-5.42	106.71	113.38
1	C	331	THR	N-CA-C	5.36	119.13	112.59
1	A	341	VAL	CB-CA-C	-5.32	105.07	111.88
1	A	184	LYS	N-CA-C	-5.21	105.72	111.71
1	A	167	SER	N-CA-C	-5.21	102.78	110.48
1	B	423	LEU	N-CA-C	-5.21	105.78	111.82
1	A	318	VAL	N-CA-C	-5.07	106.99	113.22

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	2176	0	2009	171	0
1	B	2120	0	1891	162	0
1	C	2082	0	1867	196	0
2	A	27	0	12	4	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
All	All	6415	0	5779	519	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 43.

All (519) 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:149:VAL:HG13	1:B:271:LEU:HD12	1.29	1.14
1:C:124:LEU:HB3	1:C:196:SER:HB3	1.34	1.05
1:C:146:LYS:HA	1:C:150:ILE:HD13	1.36	1.04
1:B:172:TYR:HB2	1:B:279:PRO:HG3	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:THR:HG22	1:B:414:ARG:H	1.29	0.94
1:C:238:THR:HG21	1:C:283:ASP:HB2	1.54	0.90
1:B:359:HIS:HB2	1:B:377:SER:HA	1.55	0.88
1:B:280:TRP:H	1:B:280:TRP:CD1	1.94	0.84
1:A:330:MET:HE1	1:A:407:LEU:HD23	1.61	0.83
1:A:130:VAL:HG23	1:A:185:ALA:HA	1.60	0.82
1:B:130:VAL:HG23	1:B:185:ALA:HA	1.59	0.82
1:B:170:LEU:HD11	1:B:276:THR:HG22	1.62	0.82
1:C:337:SER:O	1:C:341:VAL:HG23	1.80	0.81
1:C:258:VAL:HB	1:C:259:GLN:NE2	1.95	0.81
1:B:128:PRO:HD3	1:B:194:PHE:HB2	1.63	0.81
1:A:132:TRP:CE2	1:A:189:GLU:HG3	2.16	0.80
1:A:422:LEU:O	1:A:422:LEU:HD23	1.82	0.80
1:C:282:LEU:HD23	1:C:287:ARG:HB2	1.61	0.80
1:A:320:THR:HG22	1:A:322:GLU:H	1.46	0.78
1:C:195:PHE:HE2	1:C:217:LEU:HG	1.46	0.78
1:C:172:TYR:HB2	1:C:279:PRO:HG3	1.65	0.78
1:C:143:GLU:HA	1:C:146:LYS:HE3	1.66	0.77
1:C:316:PRO:O	1:C:401:LEU:HD12	1.85	0.77
1:A:146:LYS:HA	1:A:150:ILE:HD13	1.65	0.77
1:B:201:ASP:HB3	1:B:206:TRP:HD1	1.49	0.76
1:A:355:GLN:NE2	1:C:147:GLU:HB3	2.01	0.75
1:B:413:THR:HG22	1:B:414:ARG:N	2.01	0.75
1:C:192:SER:HA	1:C:226:PRO:HG2	1.67	0.75
1:C:231:ILE:O	1:C:234:VAL:HG13	1.87	0.75
1:C:125:SER:HB3	1:C:195:PHE:CE1	2.22	0.74
1:C:251:ARG:C	1:C:253:LYS:H	1.95	0.74
1:B:219:ALA:O	1:B:223:GLU:HG2	1.86	0.74
1:A:145:LEU:HD13	1:A:186:VAL:CG2	2.18	0.73
1:A:260:MET:C	1:A:262:GLY:H	1.97	0.73
1:B:418:ASN:OD1	1:B:420:ASP:HB3	1.88	0.73
1:C:214:VAL:HG11	1:C:256:LEU:HA	1.71	0.72
1:C:155:PHE:N	1:C:156:PRO:HD3	2.04	0.72
1:A:396:LEU:HD12	1:A:397:LYS:N	2.03	0.72
1:A:351:ILE:O	1:A:355:GLN:HG3	1.89	0.72
1:A:404:LYS:HA	1:A:407:LEU:HD12	1.70	0.72
1:C:298:LEU:HD12	1:C:298:LEU:H	1.53	0.71
1:C:404:LYS:HA	1:C:407:LEU:HD12	1.72	0.71
1:A:225:LYS:HD3	1:A:269:GLY:HA3	1.71	0.71
1:B:169:ILE:HB	1:B:273:LEU:HD23	1.70	0.71
1:C:218:PHE:CD2	1:C:259:GLN:HG3	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:MET:HE3	1:A:272:VAL:HB	1.73	0.71
1:C:259:GLN:NE2	1:C:259:GLN:H	1.88	0.71
1:A:280:TRP:H	1:A:280:TRP:CD1	2.07	0.71
1:C:203:VAL:HG13	1:C:207:MET:SD	2.30	0.70
1:A:298:LEU:HD21	1:A:417:VAL:HG21	1.71	0.70
1:C:305:THR:HG23	1:C:324:TYR:HB3	1.73	0.70
1:B:174:PRO:N	1:B:425:GLN:HE22	1.89	0.70
1:C:418:ASN:ND2	1:C:420:ASP:HB2	2.07	0.70
1:B:198:SER:O	1:B:202:LEU:HD13	1.91	0.70
1:C:354:ILE:HD12	1:C:355:GLN:N	2.06	0.70
1:A:294:ILE:HD12	1:A:294:ILE:N	2.07	0.70
1:B:280:TRP:H	1:B:280:TRP:HD1	1.38	0.70
1:C:318:VAL:HG21	1:C:400:ASP:HB3	1.74	0.70
1:A:154:LYS:C	1:A:156:PRO:HD3	2.16	0.70
1:B:374:THR:HG23	1:B:375:PRO:HD2	1.73	0.69
1:C:214:VAL:CG2	1:C:255:GLU:HG3	2.23	0.69
1:A:172:TYR:HB2	1:A:279:PRO:HG3	1.73	0.69
1:C:259:GLN:H	1:C:259:GLN:CD	2.00	0.69
1:A:283:ASP:OD2	1:A:285:ALA:HB3	1.94	0.68
1:C:145:LEU:HD22	1:C:186:VAL:HG21	1.76	0.67
1:C:374:THR:OG1	1:C:375:PRO:HD2	1.94	0.67
1:A:350:PRO:HB3	1:A:399:PRO:HG2	1.76	0.67
1:C:168:GLY:HA2	1:C:272:VAL:HB	1.76	0.67
1:B:406:PHE:O	1:B:410:ILE:HG13	1.94	0.67
1:C:149:VAL:HG13	1:C:271:LEU:HD21	1.77	0.67
1:A:174:PRO:HG3	1:A:298:LEU:HD11	1.76	0.66
1:A:199:SER:HB2	1:A:232:ASP:O	1.95	0.66
1:C:230:PHE:HA	1:C:273:LEU:O	1.95	0.66
1:C:143:GLU:O	1:C:147:GLU:HG3	1.95	0.66
1:C:304:ARG:HD2	1:C:331:THR:HB	1.75	0.66
1:A:234:VAL:HG23	1:A:282:LEU:HD13	1.77	0.66
1:A:433:GLY:O	1:A:435:GLU:N	2.29	0.66
1:B:168:GLY:HA3	1:B:290:PHE:HA	1.77	0.66
1:C:290:PHE:C	1:C:292:ARG:H	2.04	0.66
1:C:146:LYS:HA	1:C:150:ILE:CD1	2.19	0.66
1:A:151:LEU:HB3	1:A:152:PRO:HD3	1.77	0.66
1:A:249:SER:HA	1:A:252:ILE:HD13	1.77	0.65
1:C:195:PHE:CE2	1:C:217:LEU:HG	2.31	0.65
1:B:170:LEU:HD11	1:B:276:THR:CG2	2.25	0.65
1:C:143:GLU:OE2	1:C:146:LYS:HE3	1.97	0.65
1:A:158:LEU:CD2	1:B:398:GLU:HB2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:TRP:HH2	1:B:186:VAL:HG22	1.62	0.65
1:A:320:THR:HG22	1:A:322:GLU:N	2.12	0.64
1:A:215:LYS:HE3	1:A:255:GLU:OE1	1.97	0.64
1:A:396:LEU:HD12	1:A:397:LYS:H	1.60	0.64
1:B:151:LEU:C	1:B:151:LEU:HD23	2.22	0.64
1:A:319:LEU:HB3	1:A:324:TYR:CE1	2.31	0.64
1:A:174:PRO:HG3	1:A:298:LEU:CD1	2.28	0.63
1:A:188:THR:O	1:A:190:ALA:N	2.31	0.63
1:A:147:GLU:HB3	1:B:355:GLN:NE2	2.13	0.63
1:C:229:ILE:HD12	1:C:229:ILE:H	1.62	0.63
1:B:220:MET:O	1:B:224:ASN:HB2	1.98	0.63
1:C:231:ILE:HB	1:C:234:VAL:HG12	1.80	0.63
1:A:128:PRO:HG3	1:A:187:ALA:CB	2.29	0.63
1:C:214:VAL:HG21	1:C:255:GLU:HG3	1.80	0.63
1:B:232:ASP:HB3	1:B:233:GLN:NE2	2.13	0.63
1:C:351:ILE:O	1:C:355:GLN:HG3	1.99	0.63
1:B:287:ARG:HH22	1:B:433:GLY:HA3	1.62	0.62
1:B:172:TYR:HB2	1:B:279:PRO:CG	2.25	0.62
1:A:190:ALA:O	1:A:191:ASN:C	2.43	0.62
1:B:154:LYS:HG3	1:B:155:PHE:CE1	2.35	0.62
1:B:423:LEU:C	1:B:425:GLN:H	2.06	0.62
1:B:172:TYR:CB	1:B:279:PRO:HG3	2.28	0.62
1:C:231:ILE:HB	1:C:234:VAL:CG1	2.30	0.62
1:B:188:THR:C	1:B:190:ALA:H	2.07	0.61
1:A:252:ILE:HD12	1:A:252:ILE:N	2.15	0.61
1:C:218:PHE:CE2	1:C:259:GLN:HG3	2.35	0.61
1:B:311:ASN:ND2	1:B:340:ALA:HA	2.15	0.61
1:C:198:SER:C	1:C:200:SER:H	2.07	0.61
1:A:402:THR:O	1:A:405:ASP:HB2	2.01	0.61
1:C:236:ALA:O	1:C:237:LEU:HD23	2.00	0.61
1:C:311:ASN:HB3	1:C:343:VAL:HG11	1.82	0.61
1:C:319:LEU:HD21	1:C:403:ILE:HA	1.82	0.61
1:C:213:LEU:HA	1:C:216:GLN:HG3	1.83	0.61
1:B:201:ASP:HB3	1:B:206:TRP:CD1	2.34	0.60
1:B:413:THR:CG2	1:B:414:ARG:H	2.09	0.60
1:A:132:TRP:CD2	1:A:189:GLU:HG3	2.36	0.60
1:B:287:ARG:HH12	1:B:434:GLN:N	1.98	0.60
1:B:132:TRP:CH2	1:B:186:VAL:HG22	2.37	0.60
1:B:382:GLY:O	1:B:383:ALA:HB2	2.01	0.60
1:B:287:ARG:HH11	1:B:287:ARG:HG2	1.66	0.60
1:C:230:PHE:HB2	1:C:273:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:LEU:CB	1:C:196:SER:HB3	2.22	0.60
1:A:317:SER:HB2	1:A:401:LEU:HB2	1.84	0.59
1:B:175:PRO:HB3	1:B:277:ASN:ND2	2.16	0.59
1:C:229:ILE:CD1	1:C:272:VAL:HA	2.32	0.59
1:A:320:THR:HG22	1:A:321:LYS:N	2.17	0.59
1:B:187:ALA:HB2	1:B:228:ILE:HD12	1.83	0.59
1:C:290:PHE:O	1:C:292:ARG:N	2.35	0.59
1:B:122:ALA:O	1:B:124:LEU:N	2.35	0.59
1:C:150:ILE:HD12	1:C:150:ILE:N	2.18	0.59
1:C:213:LEU:HA	1:C:216:GLN:HE21	1.67	0.59
1:B:318:VAL:HG12	1:B:318:VAL:O	2.00	0.59
1:C:229:ILE:HD11	1:C:272:VAL:HA	1.83	0.59
1:A:138:LEU:O	1:A:142:LYS:HG3	2.03	0.59
1:A:280:TRP:C	1:A:282:LEU:H	2.10	0.59
1:C:306:THR:O	1:C:310:ILE:HG13	2.02	0.59
1:A:420:ASP:C	1:A:422:LEU:H	2.10	0.58
1:B:382:GLY:O	1:B:383:ALA:CB	2.50	0.58
1:B:283:ASP:OD2	1:B:286:ILE:N	2.31	0.58
1:B:378:PRO:C	1:B:380:ASP:H	2.12	0.58
1:A:301:LEU:HG	1:A:325:ARG:NH2	2.19	0.58
1:A:365:THR:C	1:A:367:ASP:H	2.10	0.58
1:C:360:PHE:O	1:C:383:ALA:HA	2.02	0.58
1:A:300:ASP:O	1:A:304:ARG:HG3	2.04	0.58
1:B:235:ASP:OD2	1:B:278:ILE:HD12	2.04	0.58
1:C:280:TRP:CD1	1:C:280:TRP:H	2.20	0.58
1:C:318:VAL:CG2	1:C:400:ASP:HB3	2.34	0.57
1:B:207:MET:HE3	1:B:207:MET:O	2.04	0.57
1:B:231:ILE:HG22	1:B:234:VAL:HG12	1.86	0.57
1:C:132:TRP:NE1	1:C:189:GLU:HG3	2.20	0.57
1:A:320:THR:CG2	1:A:321:LYS:N	2.68	0.57
1:B:151:LEU:HB3	1:B:152:PRO:HD3	1.85	0.57
1:C:193:THR:H	1:C:227:SER:HA	1.69	0.57
1:A:150:ILE:HD12	1:A:150:ILE:N	2.20	0.57
1:A:179:LYS:HB2	2:A:800:ADP:O1B	2.05	0.57
1:A:365:THR:O	1:A:367:ASP:N	2.38	0.57
1:A:351:ILE:HD11	1:C:163:ARG:HD2	1.86	0.56
1:A:151:LEU:CB	1:A:152:PRO:HD3	2.34	0.56
1:A:388:TRP:CE3	1:C:151:LEU:HD21	2.40	0.56
1:C:195:PHE:HE2	1:C:217:LEU:CG	2.18	0.56
1:A:294:ILE:HD12	1:A:294:ILE:H	1.69	0.56
1:B:364:SER:HB3	1:B:372:LYS:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:THR:C	1:C:404:LYS:H	2.13	0.56
1:A:234:VAL:HG23	1:A:282:LEU:CD1	2.34	0.56
1:B:287:ARG:HH12	1:B:434:GLN:H	1.53	0.56
1:C:258:VAL:C	1:C:260:MET:H	2.14	0.56
1:A:136:ALA:HB2	1:A:307:MET:HE3	1.88	0.55
1:A:182:LEU:O	1:A:185:ALA:HB3	2.06	0.55
1:A:349:GLN:HG3	1:A:405:ASP:OD2	2.05	0.55
1:B:145:LEU:HD13	1:B:186:VAL:CG2	2.37	0.55
1:C:140:GLY:O	1:C:141:ALA:C	2.49	0.55
1:C:199:SER:OG	1:C:237:LEU:HD21	2.05	0.55
1:C:141:ALA:O	1:C:145:LEU:HD12	2.07	0.55
1:B:132:TRP:CD1	1:B:189:GLU:HG3	2.42	0.55
1:B:423:LEU:C	1:B:425:GLN:N	2.64	0.55
1:C:287:ARG:HG2	1:C:293:ARG:HH21	1.72	0.55
1:B:280:TRP:CD1	1:B:280:TRP:N	2.68	0.55
1:C:150:ILE:O	1:C:153:VAL:HG22	2.07	0.55
1:B:402:THR:HG22	1:B:403:ILE:N	2.22	0.55
1:C:253:LYS:C	1:C:255:GLU:H	2.14	0.55
1:A:173:GLY:O	1:A:277:ASN:HA	2.07	0.55
1:B:393:ALA:C	1:B:395:GLU:H	2.15	0.55
1:C:324:TYR:O	1:C:327:LEU:N	2.40	0.54
1:A:130:VAL:HG23	1:A:185:ALA:CA	2.35	0.54
1:A:349:GLN:HE22	1:A:352:ARG:NH1	2.06	0.54
1:A:354:ILE:HA	1:A:357:ALA:HB2	1.89	0.54
1:C:354:ILE:HD12	1:C:354:ILE:C	2.32	0.54
1:C:278:ILE:HG23	1:C:280:TRP:CE2	2.42	0.54
1:C:188:THR:C	1:C:190:ALA:H	2.15	0.54
1:B:179:LYS:HE2	1:B:276:THR:O	2.08	0.54
1:A:199:SER:O	1:A:203:VAL:HG23	2.08	0.54
1:C:301:LEU:HA	1:C:304:ARG:NH2	2.22	0.54
1:A:187:ALA:HA	1:A:228:ILE:HD12	1.90	0.54
1:A:351:ILE:CD1	1:C:163:ARG:HD2	2.38	0.54
1:B:231:ILE:CG2	1:B:234:VAL:HG12	2.38	0.54
1:B:287:ARG:HG2	1:B:287:ARG:NH1	2.22	0.54
1:B:215:LYS:HA	1:B:259:GLN:HE21	1.72	0.53
1:C:125:SER:O	1:C:126:GLU:HB3	2.09	0.53
1:A:128:PRO:HG3	1:A:187:ALA:HB1	1.89	0.53
1:C:213:LEU:O	1:C:216:GLN:HB2	2.08	0.53
1:C:402:THR:C	1:C:404:LYS:N	2.66	0.53
1:A:294:ILE:HG22	1:A:295:TYR:N	2.24	0.53
1:B:279:PRO:HD2	1:B:280:TRP:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:VAL:O	1:B:318:VAL:CG1	2.55	0.53
1:A:227:SER:OG	1:A:270:VAL:HG22	2.08	0.53
1:A:260:MET:C	1:A:262:GLY:N	2.63	0.53
1:A:260:MET:O	1:A:262:GLY:N	2.33	0.53
1:B:402:THR:HG22	1:B:403:ILE:H	1.73	0.53
1:C:130:VAL:H	1:C:188:THR:HG21	1.74	0.53
1:C:190:ALA:O	1:C:191:ASN:C	2.52	0.53
1:C:230:PHE:HE1	1:C:275:ALA:CB	2.22	0.53
1:A:256:LEU:HD22	1:A:260:MET:HG3	1.90	0.53
1:A:379:GLY:HA2	1:A:383:ALA:HB2	1.90	0.53
1:B:143:GLU:HG3	1:B:147:GLU:OE2	2.09	0.53
1:B:231:ILE:O	1:B:234:VAL:HG13	2.09	0.53
1:A:128:PRO:HG3	1:A:187:ALA:HB3	1.91	0.52
1:C:155:PHE:N	1:C:156:PRO:CD	2.72	0.52
1:A:327:LEU:HD23	1:A:327:LEU:N	2.24	0.52
1:A:298:LEU:CD2	1:A:417:VAL:HG21	2.36	0.52
1:C:256:LEU:C	1:C:258:VAL:N	2.67	0.52
1:B:429:THR:O	1:B:432:PHE:HE2	1.92	0.52
1:A:365:THR:C	1:A:367:ASP:N	2.68	0.52
1:B:130:VAL:HG23	1:B:130:VAL:O	2.09	0.52
1:C:218:PHE:O	1:C:222:ARG:HB2	2.09	0.52
1:B:210:SER:C	1:B:212:LYS:H	2.17	0.52
1:B:348:MET:SD	1:B:351:ILE:HD12	2.50	0.52
1:C:143:GLU:HA	1:C:146:LYS:CE	2.37	0.52
1:C:150:ILE:O	1:C:151:LEU:C	2.53	0.52
1:C:152:PRO:HG3	1:C:159:PHE:CE2	2.45	0.52
1:C:258:VAL:HB	1:C:259:GLN:HE22	1.70	0.52
1:A:280:TRP:O	1:A:282:LEU:N	2.43	0.52
1:A:380:ASP:O	1:A:382:GLY:N	2.33	0.52
1:C:150:ILE:CD1	1:C:150:ILE:N	2.72	0.52
1:A:380:ASP:C	1:A:382:GLY:H	2.17	0.51
1:B:359:HIS:HA	1:B:384:ILE:O	2.09	0.51
1:A:283:ASP:OD2	1:A:286:ILE:HG13	2.09	0.51
1:C:152:PRO:HA	1:C:159:PHE:CE1	2.46	0.51
1:B:228:ILE:HG21	1:B:273:LEU:HD12	1.93	0.51
1:C:334:TYR:CE1	1:C:415:PRO:HG3	2.46	0.51
1:C:151:LEU:HB2	1:C:152:PRO:HD3	1.91	0.51
1:C:180:SER:HA	1:C:230:PHE:CE2	2.46	0.51
1:C:349:GLN:N	1:C:350:PRO:HD2	2.26	0.51
1:A:433:GLY:O	1:A:434:GLN:C	2.52	0.51
1:A:151:LEU:HD12	1:B:388:TRP:CZ2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:SER:OG	1:B:319:LEU:HD22	2.11	0.50
1:C:131:LYS:HA	1:C:189:GLU:HG2	1.91	0.50
1:C:150:ILE:HG22	1:C:151:LEU:N	2.26	0.50
1:A:256:LEU:CD2	1:A:260:MET:HG3	2.40	0.50
1:A:350:PRO:CB	1:A:399:PRO:HG2	2.41	0.50
1:C:418:ASN:HD21	1:C:420:ASP:HB2	1.77	0.50
1:B:168:GLY:CA	1:B:290:PHE:HA	2.42	0.50
1:C:256:LEU:C	1:C:258:VAL:H	2.19	0.50
1:B:172:TYR:CZ	1:B:295:TYR:HB2	2.47	0.50
1:C:159:PHE:CD1	1:C:159:PHE:N	2.78	0.50
1:C:182:LEU:HD23	1:C:182:LEU:C	2.37	0.50
1:C:339:ILE:O	1:C:343:VAL:HG23	2.12	0.50
1:A:200:SER:H	1:A:233:GLN:NE2	2.09	0.50
1:A:203:VAL:HG13	1:A:207:MET:HE2	1.93	0.50
1:C:319:LEU:HD21	1:C:403:ILE:CA	2.42	0.50
1:C:393:ALA:C	1:C:395:GLU:H	2.19	0.50
1:B:354:ILE:HD11	1:B:399:PRO:HD2	1.93	0.50
1:A:249:SER:C	1:A:251:ARG:H	2.19	0.49
1:A:334:TYR:CE1	1:A:415:PRO:HG3	2.47	0.49
1:A:392:GLU:HB2	1:A:395:GLU:HG3	1.94	0.49
1:C:146:LYS:O	1:C:150:ILE:HB	2.12	0.49
1:B:192:SER:HA	1:B:226:PRO:HG2	1.94	0.49
1:C:278:ILE:HD12	1:C:278:ILE:N	2.26	0.49
1:A:222:ARG:HA	1:A:270:VAL:HG21	1.95	0.49
1:B:136:ALA:CB	1:B:307:MET:HE3	2.42	0.49
1:B:283:ASP:O	1:B:287:ARG:HB2	2.11	0.49
1:C:131:LYS:N	1:C:134:ASP:OD2	2.44	0.49
1:B:202:LEU:CD1	1:B:202:LEU:N	2.75	0.49
1:A:225:LYS:HD3	1:A:269:GLY:CA	2.39	0.49
1:B:159:PHE:CE2	1:B:165:PRO:HB3	2.48	0.49
1:B:351:ILE:O	1:B:355:GLN:HG3	2.12	0.49
1:C:197:VAL:O	1:C:197:VAL:HG22	2.13	0.49
1:B:232:ASP:HB3	1:B:233:GLN:CD	2.37	0.49
1:B:428:PHE:O	1:B:429:THR:C	2.55	0.49
1:C:198:SER:C	1:C:200:SER:N	2.69	0.49
1:B:188:THR:O	1:B:190:ALA:N	2.46	0.48
1:A:287:ARG:HG2	1:A:293:ARG:NH2	2.28	0.48
1:C:253:LYS:C	1:C:255:GLU:N	2.70	0.48
1:B:210:SER:O	1:B:212:LYS:N	2.45	0.48
1:C:323:ASP:O	1:C:326:THR:HB	2.14	0.48
1:B:173:GLY:HA2	1:B:425:GLN:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:LYS:HA	1:B:194:PHE:CE1	2.48	0.48
1:B:279:PRO:HD2	1:B:280:TRP:HD1	1.78	0.48
1:C:143:GLU:HA	1:C:143:GLU:OE2	2.13	0.48
1:A:283:ASP:OD2	1:A:286:ILE:N	2.32	0.48
1:B:187:ALA:CA	1:B:228:ILE:HD12	2.43	0.48
1:B:337:SER:O	1:B:340:ALA:HB3	2.14	0.48
1:C:166:THR:HB	1:C:291:GLU:HB2	1.95	0.48
1:C:251:ARG:O	1:C:253:LYS:N	2.47	0.48
1:C:298:LEU:HD21	1:C:417:VAL:HG21	1.95	0.48
1:C:430:ARG:C	1:C:431:ASP:OD2	2.57	0.48
1:C:145:LEU:HD22	1:C:186:VAL:CG2	2.42	0.48
1:C:326:THR:O	1:C:330:MET:HG2	2.13	0.48
1:C:159:PHE:H	1:C:159:PHE:HD1	1.62	0.48
1:A:231:ILE:HG22	1:A:234:VAL:HG12	1.96	0.47
1:C:309:GLU:HG2	1:C:324:TYR:CE2	2.49	0.47
1:C:410:ILE:O	1:C:413:THR:O	2.30	0.47
1:B:138:LEU:CD2	1:B:296:ILE:HG23	2.44	0.47
1:A:128:PRO:HD3	1:A:194:PHE:HB2	1.96	0.47
1:C:256:LEU:O	1:C:258:VAL:N	2.47	0.47
1:A:136:ALA:HB2	2:A:800:ADP:HN61	1.78	0.47
1:A:337:SER:O	1:A:340:ALA:HB3	2.15	0.47
1:A:354:ILE:HG22	1:A:375:PRO:HG3	1.94	0.47
1:C:304:ARG:HD2	1:C:331:THR:CB	2.41	0.47
1:C:344:LYS:HA	1:C:347:LEU:HD12	1.95	0.47
1:B:402:THR:HG22	1:B:404:LYS:H	1.80	0.47
1:C:254:THR:HG22	1:C:254:THR:O	2.15	0.47
1:A:169:ILE:HB	1:A:273:LEU:CD2	2.45	0.47
1:B:122:ALA:HB2	1:B:206:TRP:CE2	2.50	0.47
1:C:163:ARG:O	1:C:164:LYS:C	2.57	0.47
1:C:354:ILE:CD1	1:C:355:GLN:N	2.78	0.47
1:A:178:GLY:HA2	2:A:800:ADP:PA	2.55	0.47
1:A:365:THR:N	1:A:368:ASP:OD1	2.48	0.47
1:B:374:THR:CG2	1:B:375:PRO:HD2	2.43	0.47
1:B:429:THR:O	1:B:432:PHE:CE2	2.67	0.47
1:B:221:ALA:HB1	1:B:227:SER:OG	2.15	0.47
1:C:432:PHE:CD1	1:C:432:PHE:C	2.93	0.47
1:A:387:SER:C	1:A:389:THR:N	2.71	0.46
1:B:186:VAL:O	1:B:187:ALA:C	2.58	0.46
1:B:287:ARG:HH12	1:B:433:GLY:CA	2.28	0.46
1:A:249:SER:C	1:A:251:ARG:N	2.73	0.46
1:B:403:ILE:O	1:B:407:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:THR:O	1:C:385:GLU:HA	2.15	0.46
1:B:187:ALA:CB	1:B:228:ILE:HD12	2.45	0.46
1:B:213:LEU:O	1:B:216:GLN:HB2	2.16	0.46
1:B:217:LEU:HA	1:B:220:MET:HE3	1.97	0.46
1:C:361:LYS:HA	1:C:382:GLY:O	2.15	0.46
1:C:419:GLU:O	1:C:423:LEU:HG	2.15	0.46
1:A:186:VAL:O	1:A:187:ALA:C	2.59	0.46
1:B:151:LEU:HD23	1:B:151:LEU:O	2.15	0.46
1:A:190:ALA:O	1:A:191:ASN:O	2.33	0.46
1:A:260:MET:HE3	1:A:272:VAL:CB	2.43	0.46
1:A:279:PRO:HB2	1:A:428:PHE:CD1	2.51	0.46
1:B:217:LEU:HD21	1:B:229:ILE:HG23	1.97	0.46
1:B:427:GLN:O	1:B:428:PHE:C	2.58	0.46
1:C:418:ASN:ND2	1:C:420:ASP:OD2	2.48	0.46
1:A:306:THR:HG22	1:A:310:ILE:HG13	1.98	0.46
1:B:301:LEU:HD11	1:B:329:ALA:N	2.31	0.46
1:C:172:TYR:CZ	1:C:295:TYR:HB2	2.51	0.46
1:C:315:THR:HG21	1:C:347:LEU:CD2	2.46	0.46
1:B:137:GLY:O	1:B:138:LEU:C	2.59	0.46
1:B:349:GLN:O	1:B:350:PRO:C	2.59	0.46
1:A:279:PRO:CB	1:A:428:PHE:CD1	2.99	0.46
1:C:132:TRP:CE2	1:C:189:GLU:HG3	2.51	0.46
1:C:188:THR:C	1:C:190:ALA:N	2.74	0.46
1:C:256:LEU:C	1:C:256:LEU:HD23	2.40	0.46
1:A:163:ARG:HH12	1:B:350:PRO:HG2	1.81	0.46
1:A:232:ASP:OD2	1:A:233:GLN:N	2.49	0.46
1:B:193:THR:OG1	1:B:227:SER:HB3	2.16	0.46
1:B:347:LEU:HD23	1:B:401:LEU:HD11	1.97	0.45
1:B:293:ARG:NH2	1:B:434:GLN:O	2.48	0.45
1:C:320:THR:O	1:C:321:LYS:C	2.58	0.45
1:C:311:ASN:O	1:C:312:VAL:C	2.59	0.45
1:A:390:ASP:OD1	1:A:390:ASP:N	2.50	0.45
1:B:401:LEU:HD22	1:B:406:PHE:HE1	1.82	0.45
1:C:125:SER:O	1:C:126:GLU:CB	2.65	0.45
1:C:311:ASN:OD1	1:C:340:ALA:HA	2.17	0.45
1:A:294:ILE:CG2	1:A:295:TYR:N	2.80	0.45
1:C:172:TYR:HD1	1:C:279:PRO:HG2	1.81	0.45
1:C:257:LEU:O	1:C:261:ASN:ND2	2.50	0.45
1:A:188:THR:C	1:A:190:ALA:H	2.24	0.45
1:A:292:ARG:O	1:A:293:ARG:HG3	2.17	0.45
1:B:199:SER:OG	1:B:236:ALA:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ILE:C	1:B:254:THR:H	2.24	0.45
1:A:171:LEU:O	1:A:275:ALA:HA	2.17	0.45
1:B:172:TYR:HA	1:B:276:THR:O	2.17	0.45
1:B:219:ALA:O	1:B:222:ARG:HB3	2.16	0.45
1:A:155:PHE:N	1:A:156:PRO:HD3	2.31	0.45
1:C:172:TYR:O	1:C:295:TYR:HA	2.17	0.45
1:C:298:LEU:HD11	1:C:422:LEU:HD13	1.98	0.45
1:B:217:LEU:CD2	1:B:229:ILE:HG23	2.47	0.45
1:B:420:ASP:C	1:B:422:LEU:H	2.25	0.45
1:C:186:VAL:O	1:C:187:ALA:C	2.60	0.45
1:A:330:MET:CE	1:A:407:LEU:HD23	2.40	0.44
1:C:230:PHE:HE1	1:C:275:ALA:HB3	1.82	0.44
1:C:345:ASP:OD1	1:C:345:ASP:C	2.59	0.44
1:A:203:VAL:O	1:A:207:MET:HB2	2.17	0.44
1:A:254:THR:O	1:A:258:VAL:HG23	2.17	0.44
1:B:425:GLN:O	1:B:426:GLU:C	2.60	0.44
1:A:280:TRP:CD1	1:A:280:TRP:N	2.82	0.44
1:B:251:ARG:C	1:B:253:LYS:H	2.26	0.44
1:B:363:VAL:HG12	1:B:363:VAL:O	2.17	0.44
1:C:324:TYR:C	1:C:326:THR:N	2.74	0.44
1:C:374:THR:HG23	1:C:375:PRO:N	2.32	0.44
1:A:163:ARG:NH1	1:B:350:PRO:HG2	2.33	0.44
1:A:280:TRP:C	1:A:282:LEU:N	2.75	0.44
1:B:136:ALA:HB2	1:B:307:MET:HE3	1.98	0.44
1:B:180:SER:HA	1:B:230:PHE:CE2	2.52	0.44
1:C:145:LEU:CD1	1:C:182:LEU:HD21	2.48	0.44
1:A:380:ASP:C	1:A:382:GLY:N	2.76	0.44
1:A:178:GLY:HA2	2:A:800:ADP:O5'	2.17	0.44
1:B:294:ILE:HD12	1:B:294:ILE:N	2.33	0.44
1:C:132:TRP:HH2	1:C:186:VAL:HG22	1.83	0.44
1:C:319:LEU:HD11	1:C:403:ILE:N	2.32	0.44
1:C:320:THR:O	1:C:323:ASP:N	2.50	0.44
1:A:150:ILE:HG13	1:A:190:ALA:HB2	2.00	0.43
1:A:294:ILE:N	1:A:294:ILE:CD1	2.78	0.43
1:A:396:LEU:HD23	1:C:155:PHE:CD1	2.53	0.43
1:C:177:THR:HG21	1:C:297:PRO:O	2.18	0.43
1:A:383:ALA:O	1:A:384:ILE:CB	2.66	0.43
1:B:135:VAL:O	1:B:136:ALA:O	2.35	0.43
1:A:318:VAL:HG12	1:A:318:VAL:O	2.16	0.43
1:A:387:SER:O	1:A:388:TRP:C	2.60	0.43
1:B:122:ALA:HB2	1:B:206:TRP:NE1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:PRO:HB3	1:B:428:PHE:CZ	2.53	0.43
1:C:301:LEU:C	1:C:301:LEU:HD23	2.43	0.43
1:A:182:LEU:O	1:A:182:LEU:HD22	2.17	0.43
1:C:169:ILE:HG22	1:C:170:LEU:N	2.32	0.43
1:C:169:ILE:C	1:C:290:PHE:HD2	2.26	0.43
1:A:123:ILE:HD13	1:A:217:LEU:CA	2.49	0.43
1:A:304:ARG:NH2	1:A:328:GLY:O	2.49	0.43
1:C:207:MET:HE3	1:C:210:SER:CB	2.49	0.43
1:A:220:MET:HE3	1:A:220:MET:HB2	1.76	0.43
1:A:292:ARG:C	1:A:293:ARG:HG3	2.44	0.43
1:C:184:LYS:HA	1:C:194:PHE:CD1	2.54	0.43
1:A:145:LEU:HD13	1:A:186:VAL:HG21	1.97	0.43
1:A:387:SER:O	1:A:389:THR:N	2.52	0.43
1:B:339:ILE:O	1:B:343:VAL:HG23	2.19	0.43
1:C:154:LYS:NZ	1:C:155:PHE:CZ	2.80	0.43
1:C:256:LEU:CD2	1:C:260:MET:HG3	2.49	0.43
1:A:188:THR:C	1:A:190:ALA:N	2.77	0.43
1:A:348:MET:O	1:A:352:ARG:HG3	2.18	0.43
1:B:132:TRP:HB3	1:B:142:LYS:HD2	2.00	0.43
1:B:432:PHE:O	1:B:433:GLY:C	2.62	0.43
1:C:258:VAL:C	1:C:260:MET:N	2.75	0.43
1:A:136:ALA:CB	1:A:307:MET:HE3	2.49	0.42
1:A:255:GLU:O	1:A:259:GLN:HG2	2.19	0.42
1:A:171:LEU:HB3	1:A:179:LYS:HD3	2.01	0.42
1:C:190:ALA:O	1:C:192:SER:N	2.52	0.42
1:C:309:GLU:HG2	1:C:324:TYR:CZ	2.54	0.42
1:A:233:GLN:HE21	1:A:233:GLN:HB2	1.56	0.42
1:B:283:ASP:HB3	1:B:286:ILE:CB	2.48	0.42
1:B:305:THR:HG23	1:B:324:TYR:O	2.20	0.42
1:B:401:LEU:HD22	1:B:406:PHE:CE1	2.54	0.42
1:C:145:LEU:HD11	1:C:182:LEU:HD21	2.00	0.42
1:C:329:ALA:HB3	1:C:330:MET:HE2	2.01	0.42
1:A:146:LYS:O	1:A:150:ILE:HB	2.20	0.42
1:A:141:ALA:HB1	1:A:294:ILE:HG21	2.02	0.42
1:A:331:THR:O	1:A:334:TYR:HB2	2.19	0.42
1:A:374:THR:HG23	1:A:375:PRO:HD2	2.00	0.42
1:B:202:LEU:N	1:B:202:LEU:HD12	2.35	0.42
1:B:419:GLU:O	1:B:422:LEU:HB3	2.19	0.42
1:C:125:SER:HB3	1:C:195:PHE:HE1	1.79	0.42
1:C:393:ALA:C	1:C:395:GLU:N	2.78	0.42
1:A:160:LYS:O	1:A:161:GLY:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:PRO:HG3	1:B:187:ALA:HB3	2.01	0.42
1:B:188:THR:C	1:B:190:ALA:N	2.73	0.42
1:B:202:LEU:CD1	1:B:202:LEU:H	2.33	0.42
1:B:378:PRO:C	1:B:380:ASP:N	2.77	0.42
1:B:423:LEU:O	1:B:425:GLN:N	2.53	0.42
1:C:139:GLU:O	1:C:142:LYS:HB2	2.19	0.42
1:A:123:ILE:HD13	1:A:217:LEU:HA	2.02	0.42
1:A:200:SER:H	1:A:233:GLN:HE21	1.66	0.42
1:A:362:ASP:OD2	1:A:371:ARG:HD2	2.20	0.42
1:A:326:THR:C	1:A:328:GLY:N	2.77	0.42
1:A:403:ILE:HG22	1:A:407:LEU:HD11	2.01	0.42
1:A:420:ASP:C	1:A:422:LEU:N	2.78	0.42
1:B:174:PRO:CA	1:B:425:GLN:HE22	2.32	0.42
1:C:135:VAL:HG11	1:C:138:LEU:HD12	2.02	0.42
1:C:292:ARG:HG3	1:C:292:ARG:HH11	1.84	0.42
1:A:252:ILE:N	1:A:252:ILE:CD1	2.83	0.42
1:C:277:ASN:C	1:C:278:ILE:HD12	2.44	0.42
1:C:278:ILE:HG23	1:C:280:TRP:CD2	2.55	0.42
1:A:125:SER:O	1:A:126:GLU:HB3	2.19	0.41
1:C:126:GLU:O	1:C:194:PHE:N	2.53	0.41
1:C:301:LEU:CA	1:C:304:ARG:NH2	2.82	0.41
1:B:151:LEU:C	1:B:151:LEU:CD2	2.93	0.41
1:A:192:SER:OG	1:A:226:PRO:HB2	2.20	0.41
1:A:204:SER:C	1:A:206:TRP:H	2.28	0.41
1:A:212:LYS:O	1:A:215:LYS:N	2.53	0.41
1:A:320:THR:O	1:A:324:TYR:HD1	2.02	0.41
1:B:334:TYR:CD1	1:B:415:PRO:HG3	2.56	0.41
1:C:161:GLY:C	1:C:163:ARG:H	2.28	0.41
1:A:145:LEU:HD23	1:A:145:LEU:HA	1.92	0.41
1:B:135:VAL:O	1:B:136:ALA:C	2.63	0.41
1:C:195:PHE:HB3	1:C:229:ILE:HG22	2.02	0.41
1:A:150:ILE:HD12	1:A:150:ILE:H	1.86	0.41
1:A:212:LYS:O	1:A:213:LEU:C	2.63	0.41
1:B:298:LEU:HD23	1:B:335:SER:HA	2.03	0.41
1:B:398:GLU:HA	1:B:399:PRO:HD2	1.90	0.41
1:C:280:TRP:CD1	1:C:280:TRP:N	2.86	0.41
1:C:319:LEU:HD11	1:C:403:ILE:H	1.86	0.41
1:B:335:SER:O	1:B:336:GLY:C	2.64	0.41
1:B:159:PHE:N	1:B:159:PHE:CD1	2.89	0.41
1:B:174:PRO:O	1:B:177:THR:HG23	2.20	0.41
1:B:187:ALA:HA	1:B:228:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:LEU:O	1:B:256:LEU:HD23	2.20	0.41
1:B:301:LEU:HD12	1:B:304:ARG:NH2	2.36	0.41
1:A:201:ASP:OD2	1:A:201:ASP:N	2.52	0.41
1:B:199:SER:HB3	1:B:233:GLN:O	2.21	0.41
1:B:221:ALA:HB3	1:B:229:ILE:HD11	2.02	0.41
1:B:282:LEU:HG	1:B:283:ASP:N	2.36	0.41
1:C:141:ALA:O	1:C:144:ALA:HB3	2.20	0.41
1:C:230:PHE:CE1	1:C:275:ALA:HB3	2.55	0.41
1:C:231:ILE:CG2	1:C:234:VAL:HG12	2.50	0.41
1:A:150:ILE:O	1:A:153:VAL:HG22	2.21	0.41
1:A:293:ARG:NH2	1:A:435:GLU:HA	2.36	0.41
1:B:186:VAL:C	1:B:188:THR:N	2.79	0.41
1:B:309:GLU:HG2	1:B:324:TYR:CG	2.56	0.41
1:C:154:LYS:HZ3	1:C:155:PHE:HZ	1.63	0.41
1:A:205:LYS:O	1:A:206:TRP:CG	2.75	0.40
1:C:136:ALA:CB	1:C:307:MET:HE3	2.51	0.40
1:C:222:ARG:HH11	1:C:222:ARG:HG3	1.86	0.40
1:A:143:GLU:HA	1:A:146:LYS:HD2	2.03	0.40
1:C:130:VAL:O	1:C:130:VAL:HG23	2.20	0.40
1:C:213:LEU:CA	1:C:216:GLN:HE21	2.33	0.40
1:C:249:SER:C	1:C:251:ARG:H	2.29	0.40
1:C:228:ILE:CG2	1:C:273:LEU:HB2	2.51	0.40
1:C:172:TYR:CD1	1:C:279:PRO:HG2	2.57	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	299/355 (84%)	229 (77%)	47 (16%)	23 (8%)	1 5
1	B	297/355 (84%)	217 (73%)	60 (20%)	20 (7%)	1 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	290/355 (82%)	213 (73%)	56 (19%)	21 (7%)	1	6
All	All	886/1065 (83%)	659 (74%)	163 (18%)	64 (7%)	1	6

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ALA
1	A	189	GLU
1	A	191	ASN
1	A	197	VAL
1	A	205	LYS
1	A	378	PRO
1	A	384	ILE
1	A	434	GLN
1	B	136	ALA
1	B	211	GLU
1	B	251	ARG
1	B	376	SER
1	B	378	PRO
1	B	383	ALA
1	B	431	ASP
1	B	433	GLY
1	C	136	ALA
1	C	197	VAL
1	C	211	GLU
1	C	249	SER
1	C	253	LYS
1	C	258	VAL
1	C	291	GLU
1	A	161	GLY
1	A	366	GLU
1	A	381	ASP
1	A	383	ALA
1	B	123	ILE
1	B	162	ASN
1	B	189	GLU
1	B	205	LYS
1	B	380	ASP
1	B	432	PHE
1	C	126	GLU
1	C	168	GLY
1	C	178	GLY

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Mol	Chain	Res	Type
1	C	191	ASN
1	C	252	ILE
1	C	386	MET
1	A	261	ASN
1	A	281	GLN
1	A	382	GLY
1	A	433	GLY
1	B	191	ASN
1	B	381	ASP
1	B	394	ASP
1	C	376	SER
1	C	377	SER
1	A	188	THR
1	A	212	LYS
1	A	421	ASP
1	A	432	PHE
1	C	257	LEU
1	C	259	GLN
1	C	415	PRO
1	A	291	GLU
1	A	419	GLU
1	C	189	GLU
1	C	234	VAL
1	B	160	LYS
1	B	363	VAL
1	B	424	LYS
1	C	150	ILE
1	A	310	ILE

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	204/298 (68%)	187 (92%)	17 (8%)	10	38
1	B	192/298 (64%)	174 (91%)	18 (9%)	8	33
1	C	191/298 (64%)	169 (88%)	22 (12%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	587/894 (66%)	530 (90%)	57 (10%)	8 32

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	LEU
1	A	182	LEU
1	A	196	SER
1	A	202	LEU
1	A	233	GLN
1	A	256	LEU
1	A	280	TRP
1	A	284	SER
1	A	297	PRO
1	A	300	ASP
1	A	317	SER
1	A	325	ARG
1	A	330	MET
1	A	358	THR
1	A	390	ASP
1	A	402	THR
1	A	423	LEU
1	B	139	GLU
1	B	182	LEU
1	B	232	ASP
1	B	233	GLN
1	B	276	THR
1	B	278	ILE
1	B	280	TRP
1	B	287	ARG
1	B	306	THR
1	B	317	SER
1	B	319	LEU
1	B	337	SER
1	B	341	VAL
1	B	390	ASP
1	B	392	GLU
1	B	401	LEU
1	B	423	LEU
1	B	431	ASP
1	C	139	GLU
1	C	159	PHE

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Mol	Chain	Res	Type
1	C	163	ARG
1	C	180	SER
1	C	197	VAL
1	C	218	PHE
1	C	229	ILE
1	C	232	ASP
1	C	233	GLN
1	C	260	MET
1	C	280	TRP
1	C	283	ASP
1	C	298	LEU
1	C	312	VAL
1	C	318	VAL
1	C	327	LEU
1	C	332	GLU
1	C	335	SER
1	C	345	ASP
1	C	374	THR
1	C	402	THR
1	C	431	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	GLN
1	A	261	ASN
1	A	349	GLN
1	A	434	GLN
1	B	233	GLN
1	B	261	ASN
1	B	311	ASN
1	B	355	GLN
1	B	425	GLN
1	C	216	GLN
1	C	233	GLN
1	C	261	ASN
1	C	277	ASN

5.3.3 RNA ⓘ

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](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	C	800	-	4,4,4	1.64	0	6,6,6	0.48	0
2	ADP	A	800	-	28,29,29	1.12	2 (7%)	43,45,45	1.83	8 (18%)
3	PO4	B	800	-	4,4,4	1.63	0	6,6,6	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	800	-	-	2/16/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	ADP	C5-C4	2.37	1.43	1.39
2	A	800	ADP	PA-O3A	2.10	1.61	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	ADP	C5-C4-N3	-5.37	119.32	126.72
2	A	800	ADP	N3-C4-N9	4.71	135.18	127.17
2	A	800	ADP	N3-C2-N1	-4.68	121.50	128.58
2	A	800	ADP	C5-N7-C8	3.75	109.34	103.45
2	A	800	ADP	C2-N3-C4	3.72	120.92	111.83
2	A	800	ADP	C4-C5-N7	-2.63	107.57	110.58
2	A	800	ADP	PA-O5'-C5'	-2.41	107.53	121.35
2	A	800	ADP	N9-C8-N7	-2.13	110.92	113.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

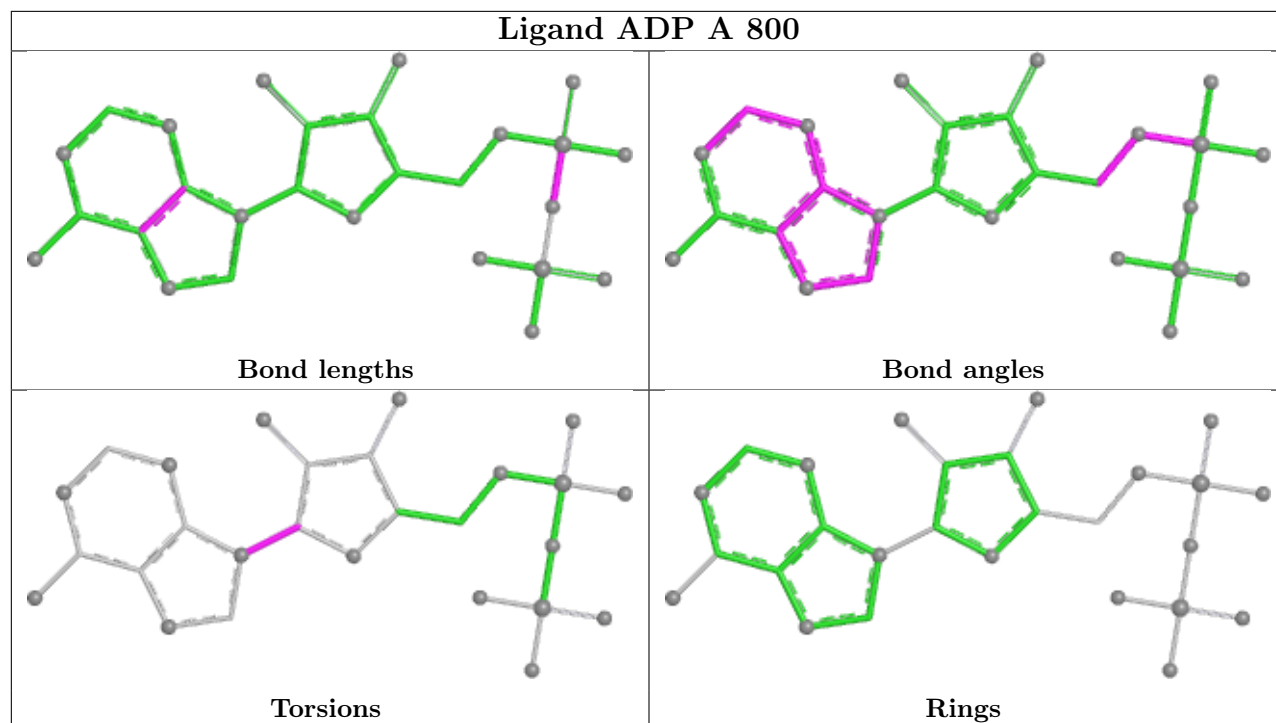
Mol	Chain	Res	Type	Atoms
2	A	800	ADP	C2'-C1'-N9-C4
2	A	800	ADP	C2'-C1'-N9-C8

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	ADP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

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	305/355 (85%)	-0.12	4 (1%) 75 55	66, 94, 139, 157	0
1	B	303/355 (85%)	0.04	9 (2%) 52 33	69, 119, 163, 184	0
1	C	296/355 (83%)	0.37	16 (5%) 31 20	97, 143, 185, 192	0
All	All	904/1065 (84%)	0.09	29 (3%) 50 31	66, 122, 174, 192	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	360	PHE	4.4
1	C	280	TRP	3.5
1	C	209	GLU	3.2
1	B	249	SER	3.1
1	B	271	LEU	2.8
1	C	272	VAL	2.8
1	C	229	ILE	2.7
1	A	432	PHE	2.6
1	B	209	GLU	2.6
1	B	202	LEU	2.6
1	C	199	SER	2.4
1	A	248	ALA	2.4
1	C	387	SER	2.4
1	C	194	PHE	2.3
1	C	256	LEU	2.3
1	A	121	SER	2.3
1	C	432	PHE	2.3
1	C	257	LEU	2.2
1	C	210	SER	2.2
1	C	249	SER	2.2
1	B	278	ILE	2.2
1	C	202	LEU	2.2
1	B	433	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	267	SER	2.2
1	C	254	THR	2.1
1	C	309	GLU	2.1
1	B	283	ASP	2.0
1	B	211	GLU	2.0
1	B	177	THR	2.0

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

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

6.3 Carbohydrates [i](#)

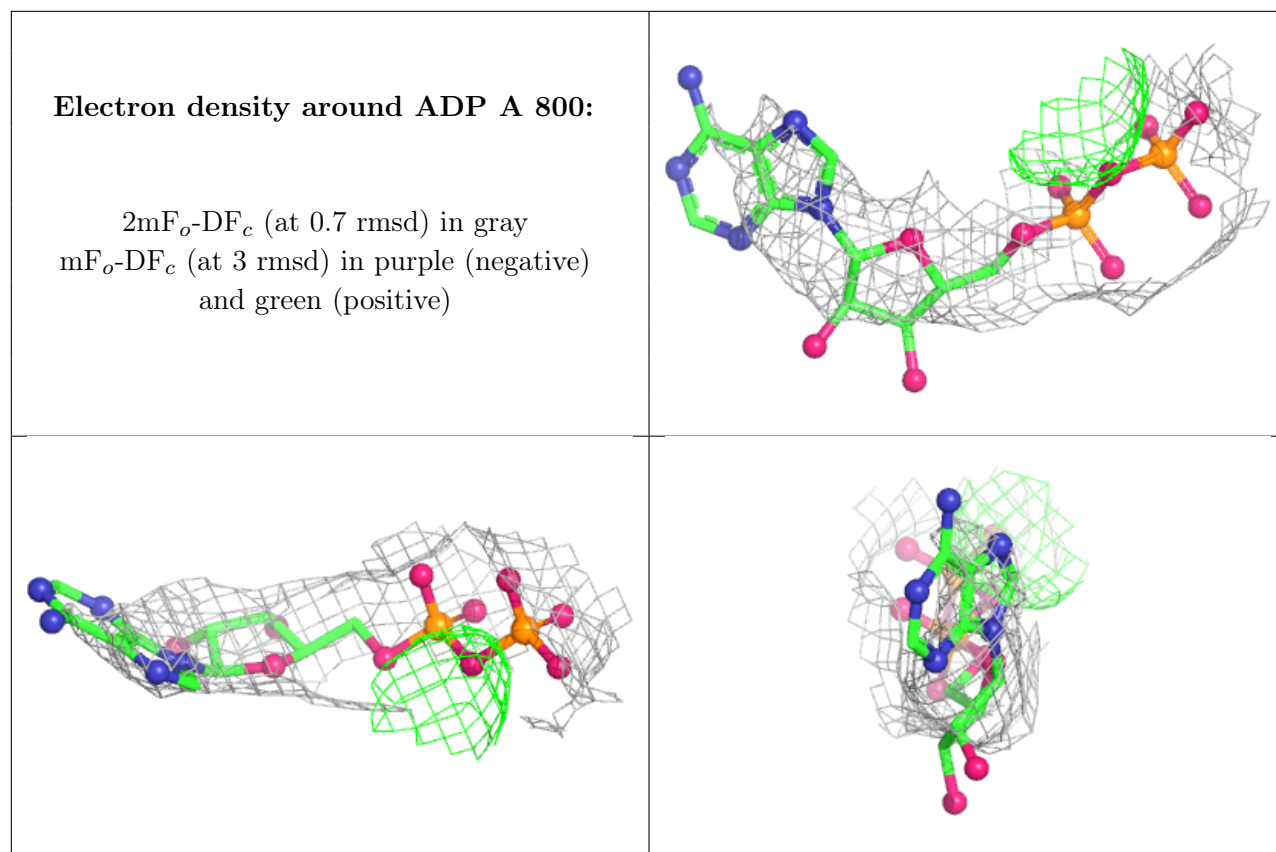
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PO4	B	800	5/5	0.66	0.14	152,152,154,155	0
3	PO4	C	800	5/5	0.79	0.10	151,151,152,152	0
2	ADP	A	800	27/27	0.85	0.14	177,179,182,183	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.