



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:59 AM UTC

PDB ID : 5L9W / pdb_00005l9w
Title : Crystal structure of the Apc core complex
Authors : Warkentin, E.; Weidenweber, S.; Ermler, U.
Deposited on : 2016-06-11
Resolution : 2.90 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

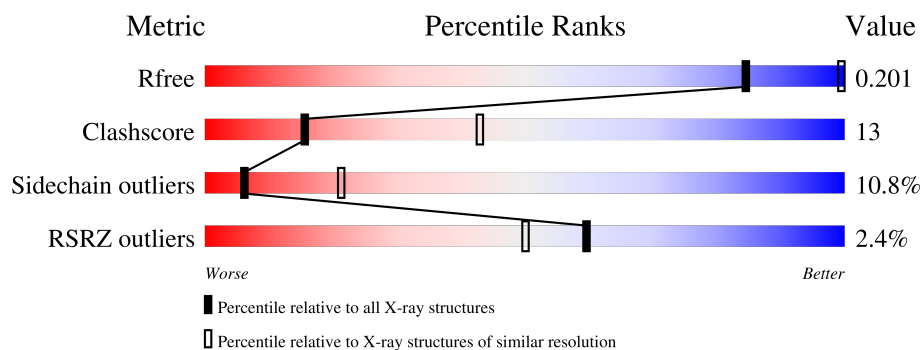
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	684	0% 70% 27% •
2	B	732	2% 67% 27% • •
3	b	658	5% 61% 32% 6% •
4	C	129	2% 63% 31% 5% •

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16761 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 Acetophenone carboxylase delta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	683	Total	C	N	O	S	0	0	0
			5285	3336	910	1002	37			

- Molecule 2 is a protein called Acetophenone carboxylase gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	711	Total	C	N	O	S	0	0	0
			5504	3490	956	1031	27			

- Molecule 3 is a protein called Acetophenone carboxylase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	b	649	Total	C	N	O	S	0	0	0
			4840	3036	849	933	22			

- Molecule 4 is a protein called Acetophenone carboxylase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	127	Total	C	N	O	S	0	0	0
			1041	663	176	196	6			

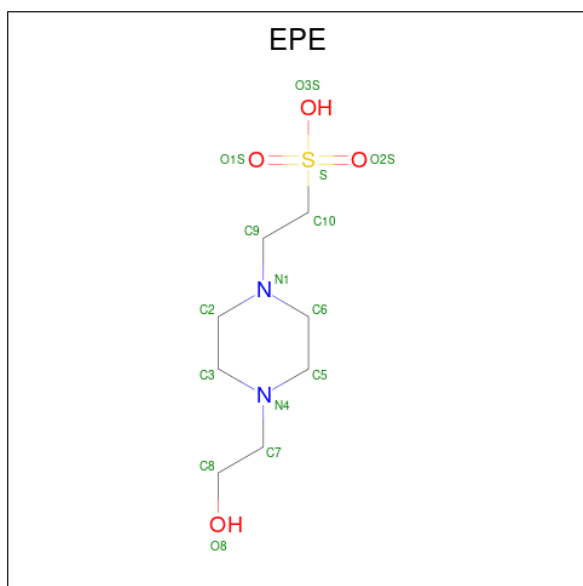
- Molecule 5 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Hg	0	0
			2	2		
5	B	1	Total	Hg	0	0
			1	1		
5	C	1	Total	Hg	0	0
			1	1		

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

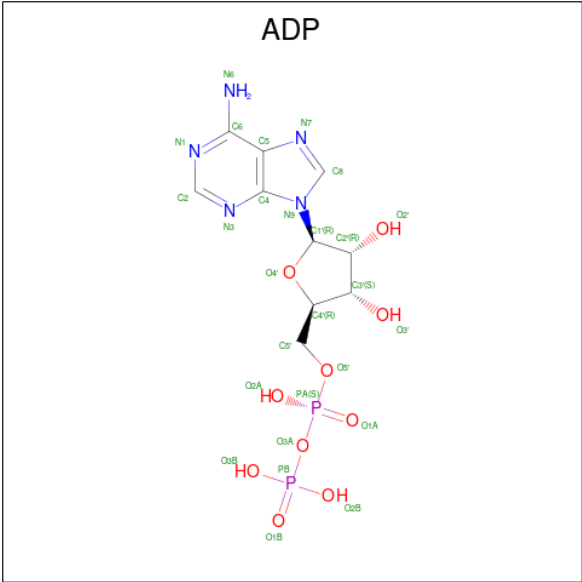
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total K 1 1	0	0

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
7	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
7	b	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

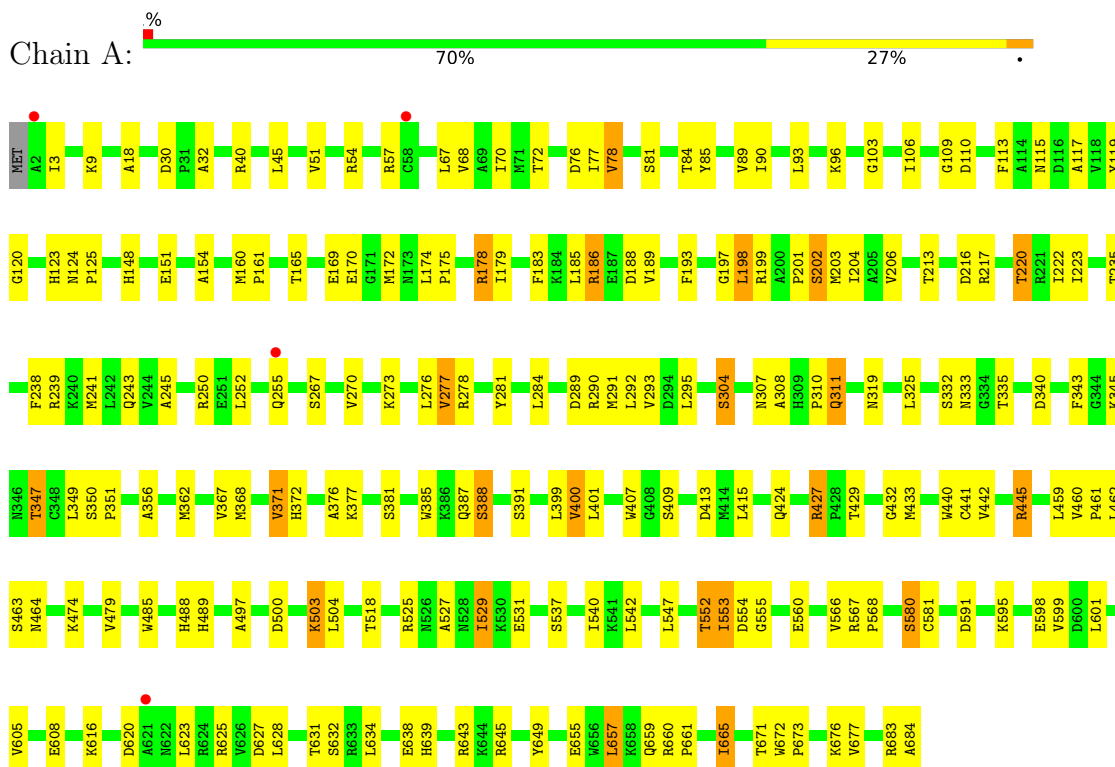
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	8	Total	O	0
			8	8	
9	B	6	Total	O	0
			6	6	

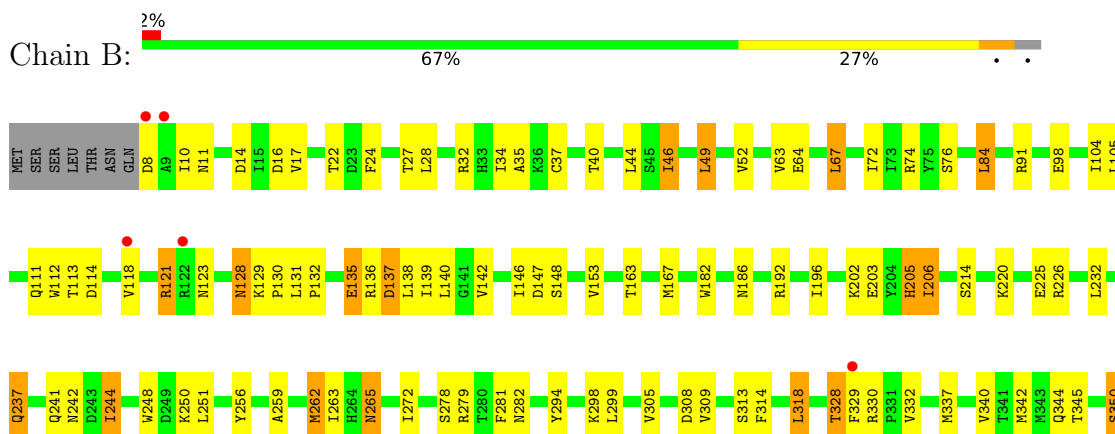
3 Residue-property plots

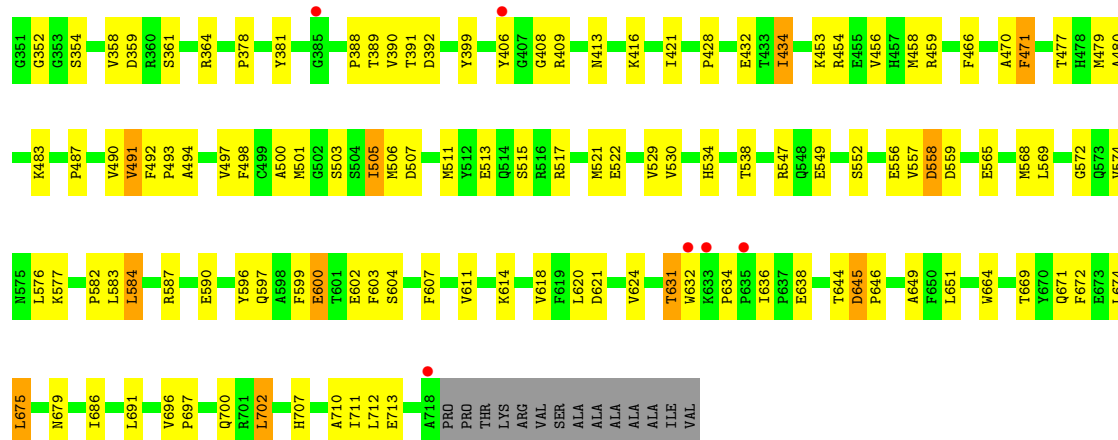
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

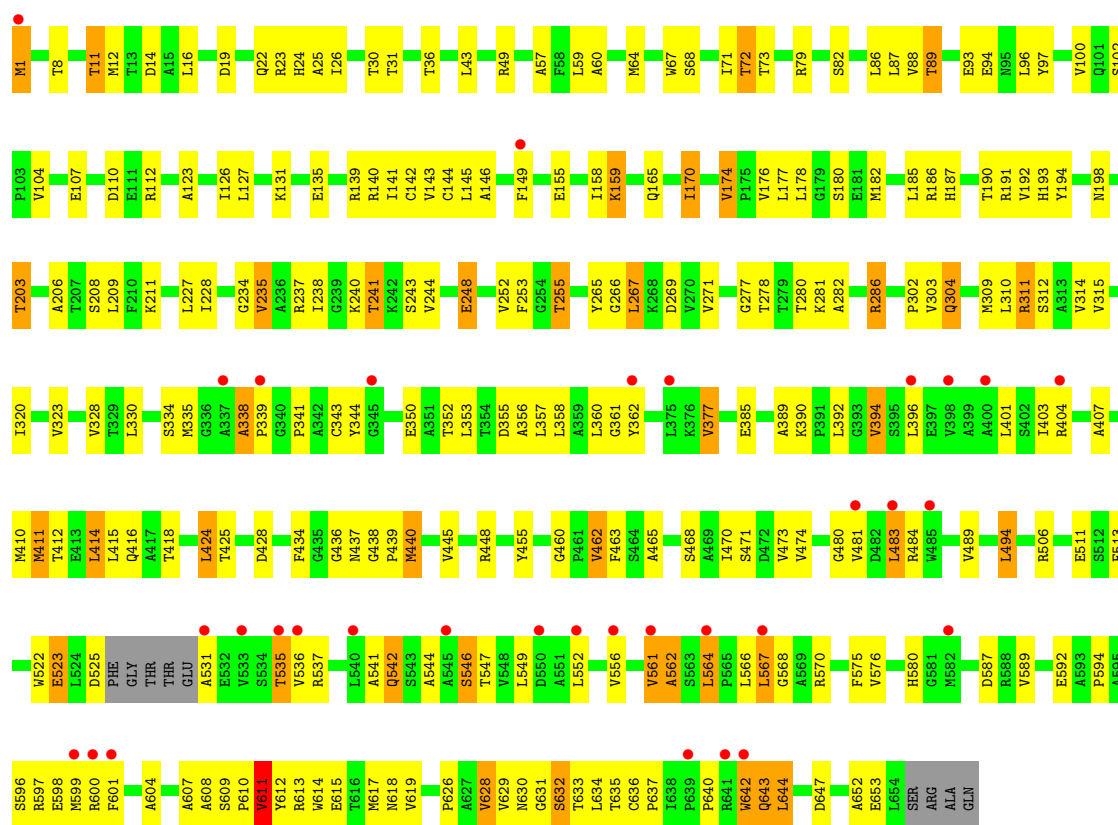


• Molecule 2: Acetophenone carboxylase gamma subunit



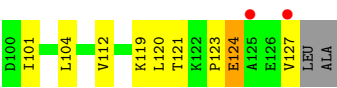


• Molecule 3: Acetophenone carboxylase alpha subunit



• Molecule 4: Acetophenone carboxylase beta subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	240.08Å 240.08Å 336.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 2.90 19.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.4 (19.97-2.90) 96.1 (19.97-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.197 , 0.235 (Not available) , 0.201	Depositor DCC
R_{free} test set	6616 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	89.7	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 76.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16761	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% 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: EPE, K, HG, ADP

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	0.42	0/5408	0.67	0/7340
2	B	0.39	0/5622	0.65	2/7627 (0.0%)
3	b	0.33	0/4925	0.63	5/6693 (0.1%)
4	C	0.31	0/1067	0.56	0/1446
All	All	0.38	0/17022	0.65	7/23106 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	b	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	b	544	ALA	CA-C-N	5.60	132.24	121.54
3	b	544	ALA	C-N-CA	5.60	132.24	121.54
2	B	645	ASP	CA-C-N	5.12	139.28	127.00
2	B	645	ASP	C-N-CA	5.12	139.28	127.00
3	b	611	VAL	CA-C-N	5.09	130.86	121.70
3	b	611	VAL	C-N-CA	5.09	130.86	121.70
3	b	338	ALA	N-CA-C	-5.07	98.61	109.81

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	b	531	ALA	Peptide
3	b	562	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	5285	0	5160	122	1
2	B	5504	0	5495	143	0
3	b	4840	0	4829	176	0
4	C	1041	0	1017	28	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	1	0	0	0	0
7	A	15	0	17	1	0
7	B	15	0	17	0	0
7	b	15	0	17	2	0
8	b	27	0	12	2	0
9	A	8	0	0	0	0
9	B	6	0	0	0	0
All	All	16761	0	16564	445	1

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 13.

All (445) 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)
3:b:642:TRP:HE3	3:b:643:GLN:H	1.17	0.90
2:B:454:ARG:HG2	2:B:458:MET:HE2	1.56	0.87
2:B:313:SER:HA	2:B:350:SER:HA	1.62	0.82
2:B:651:LEU:HD11	2:B:671:GLN:HG2	1.60	0.81
3:b:483:LEU:HD23	3:b:564:LEU:HD22	1.64	0.79
2:B:521:MET:HE2	2:B:618:VAL:HG23	1.64	0.78
1:A:525:ARG:NH2	1:A:568:PRO:O	2.18	0.77
1:A:148:HIS:HE1	1:A:160:MET:HE2	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:LYS:NZ	4:C:83:GLU:OE2	2.20	0.74
3:b:352:THR:OG1	3:b:355:ASP:OD2	2.06	0.74
3:b:208:SER:OG	7:b:802:EPE:O2S	2.06	0.73
3:b:149:PHE:HZ	3:b:480:GLY:H	1.34	0.73
3:b:596:SER:HA	3:b:610:PRO:HB3	1.73	0.71
1:A:54:ARG:HE	2:B:607:PHE:HZ	1.39	0.70
2:B:408:GLY:O	2:B:409:ARG:NH1	2.24	0.70
2:B:135:GLU:O	2:B:137:ASP:N	2.24	0.69
2:B:483:LYS:NZ	2:B:487:PRO:O	2.24	0.69
3:b:644:LEU:HD21	3:b:652:ALA:HB1	1.74	0.69
3:b:227:LEU:HB3	3:b:235:VAL:HG13	1.74	0.69
3:b:8:THR:HG23	3:b:67:TRP:HE1	1.56	0.69
3:b:155:GLU:HB3	3:b:178:LEU:HD22	1.74	0.69
3:b:626:PRO:HB3	3:b:640:PRO:HG3	1.74	0.69
2:B:490:VAL:HG22	2:B:711:ILE:HG13	1.74	0.68
2:B:577:LYS:HE3	2:B:602:GLU:HG3	1.76	0.68
1:A:529:ILE:HG12	1:A:553:ILE:HG13	1.74	0.68
3:b:14:ASP:HB3	3:b:462:VAL:HG22	1.75	0.68
2:B:14:ASP:OD1	2:B:74:ARG:NH1	2.27	0.68
2:B:282:ASN:HD21	2:B:345:THR:HG23	1.59	0.67
1:A:198:LEU:O	1:A:201:PRO:HD3	1.94	0.67
3:b:240:LYS:HD2	3:b:511:GLU:HG3	1.77	0.67
1:A:57:ARG:HD3	2:B:572:GLY:O	1.94	0.66
1:A:113:PHE:HB2	1:A:179:ILE:HD13	1.76	0.66
2:B:34:ILE:HD11	2:B:497:VAL:HG23	1.78	0.66
3:b:19:ASP:HB2	3:b:22:GLN:H	1.61	0.65
1:A:387:GLN:NE2	2:B:123:ASN:OD1	2.30	0.65
2:B:67:LEU:HG	2:B:256:TYR:HB2	1.79	0.65
3:b:96:LEU:HD22	3:b:192:VAL:HG11	1.79	0.65
1:A:148:HIS:CE1	1:A:160:MET:HE2	2.33	0.64
1:A:179:ILE:HB	1:A:189:VAL:HG11	1.80	0.64
3:b:385:GLU:HA	3:b:389:ALA:HB3	1.80	0.63
3:b:360:LEU:HD13	3:b:404:ARG:HD2	1.81	0.63
3:b:304:GLN:HE21	3:b:304:GLN:HA	1.64	0.63
1:A:415:LEU:HD12	1:A:485:TRP:CH2	2.34	0.62
2:B:278:SER:HA	2:B:281:PHE:CE2	2.34	0.62
2:B:406:TYR:C	2:B:408:GLY:H	2.07	0.62
3:b:89:THR:HG22	3:b:145:LEU:HD22	1.81	0.62
2:B:328:THR:HG21	2:B:344:GLN:HB3	1.82	0.61
3:b:11:THR:OG1	8:b:801:ADP:O1A	2.18	0.61
1:A:347:THR:HG23	1:A:349:LEU:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:VAL:O	1:A:371:VAL:HG23	2.01	0.61
3:b:536:VAL:HG22	3:b:537:ARG:H	1.65	0.61
2:B:111:GLN:HG3	2:B:130:PRO:HD2	1.82	0.61
1:A:115:ASN:ND2	1:A:172:MET:O	2.34	0.61
1:A:643:ARG:HH21	4:C:77:GLY:H	1.48	0.61
3:b:361:GLY:HA3	3:b:404:ARG:NH2	2.16	0.60
3:b:615:GLU:OE2	3:b:632:SER:OG	2.19	0.60
2:B:17:VAL:HG12	2:B:22:THR:HG23	1.84	0.60
2:B:225:GLU:N	2:B:225:GLU:OE1	2.32	0.60
3:b:356:ALA:HB2	3:b:403:ILE:HD12	1.84	0.60
1:A:239:ARG:O	1:A:243:GLN:HG3	2.02	0.60
3:b:11:THR:HG21	3:b:277:GLY:HA3	1.84	0.60
2:B:111:GLN:HG2	2:B:129:LYS:HD3	1.84	0.60
3:b:546:SER:OG	3:b:547:THR:N	2.32	0.60
1:A:407:TRP:CZ2	2:B:517:ARG:HD3	2.36	0.59
4:C:79:THR:O	4:C:79:THR:OG1	2.19	0.59
2:B:547:ARG:HG2	2:B:557:VAL:HG21	1.84	0.59
3:b:494:LEU:HD11	3:b:547:THR:HG22	1.84	0.59
2:B:568:MET:HE3	2:B:620:LEU:HB2	1.85	0.59
2:B:702:LEU:HD21	2:B:710:ALA:HB1	1.83	0.59
3:b:265:TYR:OH	3:b:647:ASP:OD2	2.13	0.59
3:b:611:VAL:HG13	3:b:628:VAL:HG12	1.84	0.59
1:A:385:TRP:CD1	4:C:119:LYS:HE3	2.36	0.59
2:B:279:ARG:HH22	2:B:511:MET:HE3	1.67	0.59
2:B:534:HIS:O	2:B:538:THR:HG23	2.03	0.59
3:b:635:THR:HG23	8:b:801:ADP:HN61	1.67	0.59
3:b:194:TYR:HE2	3:b:303:VAL:HG11	1.67	0.58
2:B:131:LEU:HD12	2:B:132:PRO:HD2	1.86	0.58
3:b:525:ASP:HB3	3:b:567:LEU:HD22	1.86	0.58
3:b:599:MET:HB2	3:b:608:ALA:HB3	1.85	0.58
2:B:24:PHE:HB3	2:B:35:ALA:HB3	1.86	0.58
3:b:592:GLU:OE1	3:b:613:ARG:NH2	2.29	0.58
1:A:527:ALA:HB1	1:A:553:ILE:HD11	1.85	0.58
1:A:347:THR:HG22	1:A:350:SER:OG	2.04	0.57
3:b:278:THR:HG22	3:b:334:SER:HB2	1.85	0.57
3:b:407:ALA:O	3:b:411:MET:HG2	2.04	0.57
2:B:52:VAL:HG12	2:B:63:VAL:HG12	1.86	0.57
1:A:115:ASN:HB3	1:A:174:LEU:H	1.70	0.57
2:B:645:ASP:HB2	2:B:646:PRO:HA	1.86	0.57
1:A:93:LEU:HD12	1:A:311:GLN:HG2	1.87	0.57
3:b:535:THR:HB	3:b:536:VAL:HB	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:415:LEU:HD12	3:b:445:VAL:HG11	1.86	0.57
2:B:163:THR:O	2:B:167:MET:HG3	2.05	0.57
3:b:311:ARG:HD2	3:b:418:THR:HG22	1.87	0.57
2:B:192:ARG:O	2:B:196:ILE:HG13	2.04	0.56
2:B:492:PHE:HD2	2:B:498:PHE:HD1	1.52	0.56
2:B:111:GLN:HE21	2:B:129:LYS:HB3	1.70	0.56
1:A:123:HIS:CD2	1:A:125:PRO:HG2	2.40	0.56
3:b:392:LEU:HB3	3:b:394:VAL:HG23	1.87	0.56
3:b:611:VAL:HA	3:b:612:TYR:HB2	1.87	0.56
3:b:619:VAL:HG13	3:b:647:ASP:O	2.06	0.56
4:C:30:ILE:HD11	4:C:38:LYS:C	2.30	0.56
2:B:517:ARG:NH1	2:B:621:ASP:OD2	2.38	0.56
1:A:276:LEU:HB2	1:A:665:ILE:HG23	1.88	0.56
3:b:440:MET:HA	3:b:637:PRO:HD3	1.87	0.56
2:B:632:TRP:C	2:B:634:PRO:HD3	2.30	0.56
4:C:72:GLU:OE1	4:C:81:GLN:NE2	2.39	0.56
1:A:72:THR:HG22	1:A:238:PHE:HB3	1.88	0.56
1:A:504:LEU:HD23	4:C:68:VAL:HB	1.88	0.56
3:b:286:ARG:HD3	3:b:424:LEU:HD21	1.88	0.56
3:b:609:SER:OG	3:b:626:PRO:O	2.22	0.56
4:C:5:ILE:HD13	4:C:120:LEU:HD21	1.86	0.56
2:B:202:LYS:O	2:B:205:HIS:HB2	2.05	0.55
1:A:284:LEU:HD11	1:A:291:MET:SD	2.46	0.55
3:b:338:ALA:HB1	3:b:339:PRO:HD2	1.89	0.55
3:b:561:VAL:HG12	3:b:562:ALA:H	1.72	0.55
1:A:503:LYS:HG2	4:C:67:TRP:CE2	2.41	0.55
4:C:24:ASP:OD2	4:C:80:ARG:NH2	2.35	0.55
1:A:110:ASP:HB2	1:A:178:ARG:HD2	1.89	0.55
1:A:113:PHE:CE2	1:A:115:ASN:HB2	2.42	0.55
3:b:434:PHE:O	3:b:438:GLY:HA3	2.08	0.54
1:A:9:LYS:NZ	1:A:311:GLN:HE21	2.05	0.54
1:A:542:LEU:HD12	2:B:98:GLU:HB3	1.90	0.54
3:b:537:ARG:HH21	3:b:570:ARG:HH12	1.56	0.54
1:A:580:SER:OG	1:A:581:CYS:N	2.36	0.54
1:A:427:ARG:NH1	1:A:432:GLY:HA2	2.23	0.54
2:B:294:TYR:CD1	2:B:505:ILE:HG12	2.43	0.54
1:A:270:VAL:HG23	1:A:273:LYS:HB2	1.90	0.54
3:b:362:TYR:CE1	3:b:597:ARG:HG2	2.43	0.54
3:b:141:ILE:HG13	3:b:174:VAL:HG11	1.90	0.54
3:b:248:GLU:HG2	3:b:310:LEU:HD23	1.90	0.53
3:b:187:HIS:CE1	3:b:304:GLN:HG3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:VAL:HG22	2:B:337:MET:HB3	1.90	0.53
1:A:77:ILE:HG23	1:A:332:SER:HA	1.90	0.53
1:A:154:ALA:HB1	1:A:161:PRO:HG3	1.90	0.53
2:B:522:GLU:HB2	2:B:529:VAL:HG21	1.91	0.53
3:b:177:LEU:HD11	3:b:182:MET:HB2	1.90	0.53
3:b:43:LEU:HD13	3:b:59:LEU:HD11	1.91	0.52
1:A:362:MET:HA	1:A:362:MET:HE2	1.90	0.52
1:A:445:ARG:HH22	2:B:114:ASP:CG	2.17	0.52
3:b:131:LYS:O	3:b:135:GLU:HG3	2.10	0.52
1:A:85:TYR:HB2	1:A:319:ASN:HA	1.91	0.52
2:B:378:PRO:HD2	2:B:381:TYR:CE1	2.45	0.52
3:b:16:LEU:HD13	3:b:462:VAL:HG11	1.92	0.52
3:b:356:ALA:O	3:b:360:LEU:HD12	2.08	0.52
1:A:78:VAL:O	1:A:241:MET:HE2	2.09	0.52
2:B:359:ASP:HB2	2:B:364:ARG:H	1.73	0.52
3:b:323:VAL:HG21	3:b:392:LEU:HD21	1.92	0.52
2:B:491:VAL:HG12	2:B:493:PRO:HD3	1.91	0.52
2:B:493:PRO:HD2	2:B:672:PHE:CZ	2.45	0.52
3:b:235:VAL:O	3:b:473:VAL:HA	2.10	0.52
3:b:252:VAL:HA	3:b:255:THR:HG23	1.91	0.52
4:C:104:LEU:HD11	4:C:120:LEU:HD11	1.91	0.52
3:b:79:ARG:HE	3:b:107:GLU:HB3	1.75	0.52
2:B:214:SER:HB2	2:B:226:ARG:HG2	1.92	0.51
2:B:556:GLU:HB2	2:B:559:ASP:OD2	2.10	0.51
3:b:412:THR:HG21	3:b:448:ARG:HB2	1.91	0.51
3:b:102:SER:OG	3:b:104:VAL:HG22	2.10	0.51
1:A:400:VAL:HA	1:A:413:ASP:O	2.11	0.51
1:A:598:GLU:OE2	1:A:625:ARG:HA	2.10	0.51
3:b:361:GLY:HA3	3:b:404:ARG:HH22	1.76	0.51
1:A:276:LEU:HD21	4:C:88:PRO:HB3	1.92	0.51
3:b:462:VAL:HG13	3:b:465:ALA:HB3	1.92	0.51
2:B:203:GLU:OE2	3:b:159:LYS:HE3	2.11	0.51
2:B:378:PRO:HD2	2:B:381:TYR:CD1	2.46	0.51
2:B:147:ASP:HB3	2:B:153:VAL:HG21	1.93	0.51
2:B:503:SER:HA	2:B:506:MET:HE2	1.93	0.51
4:C:10:TYR:CE1	4:C:80:ARG:HD3	2.46	0.50
1:A:68:VAL:CG2	1:A:81:SER:HB3	2.41	0.50
3:b:598:GLU:HA	3:b:607:ALA:HA	1.93	0.50
1:A:57:ARG:HH21	1:A:413:ASP:CG	2.20	0.50
1:A:553:ILE:HG12	1:A:554:ASP:N	2.26	0.50
1:A:649:TYR:CG	4:C:38:LYS:HA	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:599:MET:CG	3:b:608:ALA:HB3	2.42	0.50
1:A:245:ALA:HB1	1:A:335:THR:HG23	1.92	0.50
2:B:497:VAL:O	2:B:501:MET:HG3	2.12	0.49
1:A:197:GLY:O	1:A:199:ARG:N	2.45	0.49
2:B:16:ASP:HA	2:B:76:SER:O	2.11	0.49
3:b:541:ALA:C	3:b:542:GLN:HG3	2.36	0.49
1:A:560:GLU:CD	1:A:567:ARG:HH12	2.20	0.49
2:B:105:LEU:HD11	2:B:136:ARG:HB2	1.93	0.49
3:b:237:ARG:HB2	3:b:511:GLU:HG2	1.93	0.49
2:B:40:THR:HG21	2:B:46:ILE:HG22	1.95	0.49
3:b:597:ARG:NH1	3:b:598:GLU:OE1	2.46	0.49
1:A:103:GLY:HA2	1:A:106:ILE:HD12	1.94	0.49
2:B:242:ASN:ND2	3:b:139:ARG:HH22	2.10	0.49
2:B:406:TYR:O	2:B:408:GLY:N	2.45	0.49
3:b:282:ALA:O	3:b:310:LEU:HD12	2.13	0.49
4:C:11:LEU:HD11	4:C:36:TYR:CG	2.47	0.49
2:B:582:PRO:O	2:B:583:LEU:HD23	2.13	0.48
3:b:36:THR:HG21	3:b:211:LYS:HG2	1.94	0.48
1:A:310:PRO:HB3	1:A:343:PHE:CZ	2.48	0.48
2:B:596:TYR:OH	2:B:600:GLU:HG3	2.13	0.48
3:b:401:LEU:HD11	3:b:601:PHE:HD1	1.79	0.48
1:A:70:ILE:HD13	1:A:222:ILE:HD11	1.95	0.48
2:B:265:ASN:HD21	2:B:279:ARG:HA	1.79	0.48
4:C:85:GLU:HG2	4:C:87:LEU:HG	1.96	0.48
1:A:250:ARG:HG3	1:A:289:ASP:HB2	1.95	0.48
2:B:27:THR:HG22	2:B:32:ARG:HG2	1.95	0.48
2:B:644:THR:HA	2:B:679:ASN:HA	1.95	0.48
3:b:335:MET:O	3:b:338:ALA:HB3	2.14	0.48
3:b:425:THR:O	3:b:428:ASP:N	2.32	0.48
1:A:459:LEU:O	1:A:461:PRO:HD3	2.14	0.48
2:B:241:GLN:HG2	3:b:139:ARG:NH2	2.29	0.48
1:A:401:LEU:HD12	1:A:415:LEU:HD11	1.96	0.48
2:B:434:ILE:HG12	2:B:664:TRP:CZ2	2.49	0.48
2:B:568:MET:HB2	2:B:599:PHE:CE1	2.48	0.47
3:b:23:ARG:NH2	3:b:580:HIS:O	2.46	0.47
4:C:45:ARG:HG3	4:C:49:GLU:OE1	2.15	0.47
1:A:595:LYS:O	1:A:598:GLU:HB3	2.15	0.47
2:B:139:ILE:O	2:B:140:LEU:HD23	2.14	0.47
3:b:12:MET:C	3:b:30:THR:HG23	2.39	0.47
4:C:11:LEU:HD23	4:C:11:LEU:HA	1.63	0.47
1:A:18:ALA:HB2	1:A:239:ARG:CZ	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:LEU:HD11	2:B:250:LYS:HB3	1.97	0.47
1:A:500:ASP:OD1	1:A:500:ASP:N	2.47	0.47
2:B:279:ARG:NH2	2:B:511:MET:HE3	2.29	0.47
2:B:329:PHE:CD1	2:B:330:ARG:N	2.79	0.47
2:B:329:PHE:CD2	2:B:329:PHE:N	2.81	0.47
3:b:330:LEU:HB2	3:b:410:MET:HE1	1.95	0.47
2:B:305:VAL:HG22	2:B:318:LEU:HD22	1.96	0.47
2:B:413:ASN:ND2	2:B:416:LYS:HB2	2.30	0.47
2:B:494:ALA:HB1	2:B:691:LEU:HD12	1.97	0.47
3:b:180:SER:HA	3:b:191:ARG:HD2	1.96	0.47
3:b:209:LEU:HD13	3:b:228:ILE:HG12	1.96	0.47
1:A:119:TYR:CE1	1:A:175:PRO:HB3	2.50	0.47
2:B:340:VAL:O	2:B:342:MET:HG3	2.15	0.47
3:b:281:LYS:HB3	3:b:310:LEU:HD11	1.97	0.47
3:b:525:ASP:O	3:b:566:LEU:HD22	2.15	0.47
3:b:589:VAL:O	3:b:618:ASN:ND2	2.41	0.47
3:b:309:MET:HG2	3:b:311:ARG:HH12	1.79	0.47
3:b:357:LEU:HD13	3:b:440:MET:SD	2.55	0.47
3:b:439:PRO:HB2	3:b:636:CYS:HB2	1.97	0.47
3:b:594:PRO:HB2	3:b:610:PRO:HG2	1.95	0.47
2:B:72:ILE:HD12	2:B:259:ALA:HB3	1.97	0.47
2:B:493:PRO:HD2	2:B:672:PHE:CE2	2.50	0.47
1:A:165:THR:N	1:A:169:GLU:OE1	2.32	0.46
1:A:57:ARG:HG2	1:A:203:MET:HG3	1.96	0.46
1:A:202:SER:HB2	7:A:704:EPE:O3S	2.15	0.46
1:A:424:GLN:OE1	1:A:427:ARG:NH1	2.47	0.46
2:B:352:GLY:HA3	2:B:391:THR:HG23	1.98	0.46
3:b:159:LYS:HD2	3:b:176:VAL:HB	1.97	0.46
2:B:358:VAL:HG11	2:B:428:PRO:HB2	1.97	0.46
3:b:228:ILE:HB	3:b:241:THR:HG21	1.97	0.46
1:A:30:ASP:OD1	1:A:32:ALA:N	2.49	0.46
1:A:308:ALA:O	1:A:351:PRO:HD3	2.15	0.46
1:A:474:LYS:HD2	1:A:591:ASP:OD2	2.16	0.46
3:b:144:CYS:CB	3:b:192:VAL:HG22	2.46	0.46
2:B:131:LEU:HD12	2:B:132:PRO:CD	2.46	0.46
1:A:267:SER:HB3	1:A:277:VAL:HG22	1.97	0.46
1:A:639:HIS:ND1	4:C:78:CYS:O	2.48	0.46
3:b:269:ASP:HB3	3:b:424:LEU:CD1	2.46	0.46
3:b:353:LEU:HD13	3:b:403:ILE:HG22	1.97	0.46
3:b:611:VAL:HG11	3:b:630:ASN:HB2	1.97	0.46
1:A:433:MET:SD	2:B:128:ASN:HA	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:ASN:ND2	2:B:279:ARG:HA	2.31	0.46
3:b:523:GLU:HG2	3:b:570:ARG:HH21	1.81	0.46
3:b:110:ASP:OD2	3:b:112:ARG:HD2	2.16	0.45
1:A:660:ARG:HG2	1:A:661:PRO:O	2.16	0.45
3:b:96:LEU:HA	3:b:96:LEU:HD23	1.79	0.45
3:b:72:THR:HG21	3:b:243:SER:O	2.15	0.45
2:B:697:PRO:HD2	2:B:700:GLN:HG3	1.99	0.45
1:A:76:ASP:OD1	1:A:96:LYS:NZ	2.43	0.45
1:A:385:TRP:O	1:A:388:SER:OG	2.34	0.45
2:B:480:ALA:HB2	2:B:712:LEU:HD21	1.98	0.45
3:b:522:TRP:CZ2	3:b:549:LEU:HD13	2.51	0.45
1:A:170:GLU:OE1	1:A:356:ALA:HB1	2.16	0.45
1:A:290:ARG:NH1	1:A:340:ASP:OD2	2.49	0.45
2:B:491:VAL:CG1	2:B:493:PRO:HD3	2.46	0.45
3:b:86:LEU:HA	3:b:86:LEU:HD23	1.69	0.45
3:b:604:ALA:HB1	3:b:608:ALA:HB2	1.99	0.45
2:B:492:PHE:CD2	2:B:498:PHE:HD1	2.33	0.45
2:B:503:SER:HA	2:B:506:MET:CE	2.47	0.45
1:A:188:ASP:N	1:A:188:ASP:OD1	2.49	0.45
1:A:372:HIS:O	1:A:376:ALA:HB2	2.17	0.45
1:A:399:LEU:HD23	1:A:497:ALA:HB2	1.98	0.45
2:B:675:LEU:HB2	2:B:679:ASN:OD1	2.16	0.45
3:b:1:MET:HE2	3:b:1:MET:HB3	1.73	0.45
1:A:40:ARG:HD2	1:A:40:ARG:HA	1.74	0.44
2:B:263:ILE:HG12	2:B:506:MET:HE1	1.99	0.44
3:b:629:VAL:O	3:b:635:THR:HA	2.17	0.44
2:B:558:ASP:OD1	2:B:558:ASP:N	2.49	0.44
1:A:84:THR:HB	1:A:441:CYS:SG	2.58	0.44
1:A:172:MET:HE1	1:A:193:PHE:CE2	2.53	0.44
1:A:407:TRP:CE2	2:B:517:ARG:HD3	2.53	0.44
4:C:80:ARG:HG3	4:C:81:GLN:N	2.32	0.44
1:A:57:ARG:O	1:A:57:ARG:HG3	2.17	0.44
1:A:529:ILE:HD11	1:A:553:ILE:HG21	1.98	0.44
2:B:67:LEU:HD21	2:B:251:LEU:HD23	1.99	0.44
2:B:67:LEU:CG	2:B:256:TYR:HB2	2.47	0.44
1:A:293:VAL:HG12	1:A:295:LEU:HG	2.00	0.44
2:B:507:ASP:HA	2:B:631:THR:OG1	2.18	0.44
2:B:603:PHE:CE2	2:B:611:VAL:HG23	2.51	0.44
1:A:89:VAL:HG12	1:A:333:ASN:HA	1.99	0.44
3:b:437:ASN:O	3:b:440:MET:HB2	2.18	0.44
1:A:57:ARG:NH2	1:A:413:ASP:OD2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:PRO:HB3	2:B:421:ILE:HG12	1.99	0.44
2:B:669:THR:HA	2:B:686:ILE:O	2.18	0.44
3:b:599:MET:HE1	3:b:628:VAL:HG23	2.00	0.44
4:C:45:ARG:NE	4:C:72:GLU:OE2	2.51	0.44
1:A:304:SER:O	1:A:307:ASN:ND2	2.50	0.44
2:B:471:PHE:N	2:B:471:PHE:CD1	2.85	0.44
3:b:385:GLU:HB2	3:b:396:LEU:HD21	2.00	0.44
3:b:468:SER:O	3:b:471:SER:OG	2.24	0.44
2:B:454:ARG:O	2:B:458:MET:HG3	2.18	0.43
3:b:22:GLN:HG2	3:b:24:HIS:NE2	2.33	0.43
4:C:45:ARG:HG3	4:C:49:GLU:CD	2.42	0.43
3:b:22:GLN:HG3	3:b:23:ARG:N	2.33	0.43
3:b:234:GLY:HA3	3:b:474:VAL:HB	2.00	0.43
3:b:341:PRO:HG2	3:b:344:TYR:HE2	1.83	0.43
3:b:341:PRO:C	3:b:343:CYS:H	2.26	0.43
1:A:113:PHE:HE2	1:A:115:ASN:HB2	1.83	0.43
1:A:627:ASP:O	1:A:628:LEU:HB2	2.19	0.43
2:B:17:VAL:HG21	2:B:44:LEU:HD13	2.00	0.43
2:B:569:LEU:HG	2:B:576:LEU:HD23	2.00	0.43
1:A:109:GLY:HA2	1:A:183:PHE:CE1	2.54	0.43
3:b:25:ALA:O	3:b:49:ARG:NH1	2.51	0.43
3:b:43:LEU:HD23	3:b:43:LEU:HA	1.76	0.43
2:B:329:PHE:CG	2:B:330:ARG:N	2.87	0.43
3:b:126:ILE:HD11	3:b:158:ILE:HG12	2.00	0.43
2:B:84:LEU:HA	2:B:84:LEU:HD23	1.74	0.43
2:B:148:SER:HA	2:B:182:TRP:CE2	2.54	0.43
2:B:352:GLY:CA	2:B:391:THR:HG23	2.48	0.43
2:B:470:ALA:HB3	2:B:491:VAL:HG23	2.00	0.43
2:B:505:ILE:HA	2:B:505:ILE:HD12	1.75	0.43
3:b:567:LEU:HG	3:b:568:GLY:H	1.84	0.43
1:A:547:LEU:HD23	1:A:547:LEU:HA	1.80	0.43
1:A:595:LYS:O	1:A:599:VAL:HG23	2.19	0.43
2:B:299:LEU:HD23	2:B:299:LEU:HA	1.81	0.43
1:A:372:HIS:CD2	1:A:391:SER:HA	2.54	0.43
1:A:462:LEU:HD23	1:A:463:SER:N	2.34	0.43
3:b:614:TRP:CE3	3:b:617:MET:HE2	2.53	0.43
1:A:620:ASP:OD2	1:A:623:LEU:HD13	2.19	0.43
3:b:23:ARG:HH12	3:b:580:HIS:HB2	1.84	0.43
3:b:513:PHE:HB3	3:b:575:PHE:CZ	2.54	0.43
1:A:45:LEU:HD21	1:A:70:ILE:HG13	2.00	0.43
1:A:154:ALA:O	1:A:199:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:VAL:HA	2:B:121:ARG:HB2	2.00	0.43
4:C:123:PRO:O	4:C:124:GLU:HG2	2.17	0.43
2:B:146:ILE:HD13	2:B:186:ASN:HB3	2.01	0.42
2:B:305:VAL:HG23	2:B:466:PHE:CD1	2.53	0.42
2:B:552:SER:HB2	3:b:127:LEU:HD13	2.01	0.42
3:b:481:VAL:HG11	3:b:484:ARG:NH2	2.34	0.42
3:b:599:MET:HG3	3:b:608:ALA:HB3	2.00	0.42
1:A:672:TRP:HA	1:A:673:PRO:HA	1.79	0.42
2:B:649:ALA:HA	2:B:674:LEU:HD23	2.01	0.42
3:b:71:ILE:H	3:b:71:ILE:HG13	1.67	0.42
3:b:79:ARG:NE	3:b:107:GLU:HB3	2.34	0.42
2:B:241:GLN:HG2	3:b:139:ARG:HH21	1.84	0.42
2:B:244:ILE:HG13	2:B:272:ILE:HD11	2.02	0.42
3:b:440:MET:HB3	3:b:440:MET:HE2	1.60	0.42
4:C:5:ILE:HB	4:C:13:LEU:HB3	2.01	0.42
3:b:89:THR:CG2	3:b:146:ALA:H	2.31	0.42
3:b:127:LEU:CD1	3:b:165:GLN:HG3	2.49	0.42
4:C:20:TRP:CD1	4:C:32:ALA:HA	2.55	0.42
1:A:504:LEU:CD2	4:C:68:VAL:HB	2.50	0.42
2:B:220:LYS:HA	2:B:515:SER:OG	2.20	0.42
2:B:389:THR:O	2:B:392:ASP:HB2	2.19	0.42
3:b:412:THR:O	3:b:416:GLN:HB2	2.19	0.42
3:b:642:TRP:HE3	3:b:643:GLN:N	1.99	0.42
1:A:9:LYS:HG2	1:A:93:LEU:HD13	2.01	0.42
3:b:311:ARG:HB3	3:b:414:LEU:HD21	2.01	0.42
3:b:436:GLY:C	3:b:438:GLY:H	2.27	0.42
3:b:483:LEU:HB3	3:b:484:ARG:H	1.47	0.42
1:A:117:ALA:HA	1:A:120:GLY:O	2.20	0.42
2:B:91:ARG:HD3	2:B:138:LEU:HD11	2.01	0.42
2:B:513:GLU:HG2	2:B:624:VAL:HG13	2.02	0.42
2:B:603:PHE:HE2	2:B:611:VAL:HG23	1.85	0.42
3:b:320:ILE:HG21	3:b:350:GLU:OE1	2.20	0.42
3:b:552:LEU:HD23	3:b:552:LEU:HA	1.89	0.42
3:b:599:MET:HE3	3:b:599:MET:HB3	1.67	0.42
1:A:124:ASN:N	1:A:125:PRO:HD2	2.34	0.42
1:A:186:ARG:HB3	1:A:188:ASP:OD1	2.20	0.42
1:A:216:ASP:O	1:A:220:THR:HG23	2.20	0.42
1:A:638:GLU:OE2	1:A:645:ARG:NH2	2.52	0.42
3:b:89:THR:HG23	3:b:97:TYR:OH	2.19	0.42
3:b:123:ALA:O	3:b:127:LEU:HG	2.20	0.42
3:b:140:ARG:NH1	3:b:203:THR:OG1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:341:PRO:HB3	3:b:352:THR:HG21	2.01	0.42
3:b:636:CYS:HA	3:b:637:PRO:HD3	1.87	0.42
1:A:462:LEU:HD23	1:A:464:ASN:H	1.85	0.42
2:B:471:PHE:N	2:B:471:PHE:HD1	2.17	0.42
3:b:187:HIS:HD2	3:b:190:THR:H	1.67	0.42
2:B:84:LEU:HD11	2:B:232:LEU:HD22	2.02	0.41
3:b:341:PRO:HG2	3:b:344:TYR:CE2	2.55	0.41
3:b:455:TYR:CE1	3:b:653:GLU:HG3	2.55	0.41
3:b:599:MET:CB	3:b:608:ALA:HB3	2.48	0.41
7:b:802:EPE:H21	7:b:802:EPE:H102	1.80	0.41
2:B:565:GLU:HB2	2:B:624:VAL:HB	2.01	0.41
3:b:460:GLY:O	3:b:463:PHE:HB2	2.20	0.41
2:B:308:ASP:O	2:B:314:PHE:HA	2.20	0.41
3:b:424:LEU:O	3:b:428:ASP:HB2	2.20	0.41
3:b:562:ALA:O	3:b:564:LEU:N	2.53	0.41
2:B:359:ASP:OD2	2:B:361:SER:N	2.41	0.41
3:b:358:LEU:HG	3:b:377:VAL:HG13	2.03	0.41
3:b:481:VAL:HG11	3:b:484:ARG:CZ	2.50	0.41
1:A:643:ARG:NH2	4:C:77:GLY:H	2.14	0.41
3:b:228:ILE:HD13	3:b:238:ILE:HG12	2.03	0.41
1:A:616:LYS:O	1:A:631:THR:HG23	2.21	0.41
2:B:237:GLN:NE2	3:b:170:ILE:O	2.54	0.41
2:B:309:VAL:HG22	2:B:314:PHE:CD1	2.55	0.41
2:B:479:MET:HE2	2:B:712:LEU:HB3	2.03	0.41
2:B:497:VAL:O	2:B:500:ALA:HB3	2.20	0.41
3:b:631:GLY:N	3:b:634:LEU:O	2.42	0.41
1:A:278:ARG:HD3	1:A:281:TYR:HB2	2.03	0.41
2:B:584:LEU:HD23	2:B:584:LEU:HA	1.90	0.41
3:b:87:LEU:HD23	3:b:87:LEU:HA	1.78	0.41
1:A:199:ARG:HH11	1:A:199:ARG:HD3	1.74	0.41
1:A:252:LEU:HA	1:A:252:LEU:HD23	1.79	0.41
1:A:547:LEU:HD23	1:A:552:THR:HB	2.02	0.41
2:B:11:ASN:OD1	2:B:28:LEU:HD12	2.21	0.41
2:B:262:MET:HE2	2:B:262:MET:HB3	1.70	0.41
2:B:298:LYS:HE2	2:B:707:HIS:NE2	2.36	0.41
3:b:102:SER:OG	3:b:193:HIS:HE1	2.03	0.41
3:b:266:GLY:C	3:b:267:LEU:HD23	2.46	0.41
1:A:51:VAL:HG21	1:A:217:ARG:CZ	2.51	0.41
1:A:554:ASP:OD1	1:A:555:GLY:N	2.54	0.41
2:B:112:TRP:CE3	2:B:113:THR:HG22	2.56	0.41
3:b:193:HIS:HD2	3:b:302:PRO:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:237:ARG:O	3:b:238:ILE:C	2.63	0.41
1:A:657:LEU:HD13	1:A:657:LEU:HA	1.79	0.40
1:A:671:THR:HG22	1:A:676:LYS:N	2.36	0.40
2:B:206:ILE:HD13	3:b:206:ALA:HB2	2.03	0.40
3:b:385:GLU:O	3:b:390:LYS:HB2	2.21	0.40
3:b:437:ASN:HA	3:b:440:MET:HG3	2.02	0.40
3:b:440:MET:HA	3:b:637:PRO:CD	2.52	0.40
2:B:354:SER:HB2	2:B:390:VAL:HG23	2.03	0.40
2:B:399:TYR:HA	2:B:686:ILE:CD1	2.51	0.40
2:B:456:VAL:HG13	2:B:466:PHE:CE2	2.56	0.40
3:b:87:LEU:HB2	3:b:143:VAL:HG22	2.02	0.40
3:b:144:CYS:HB3	3:b:192:VAL:HG22	2.02	0.40
1:A:368:MET:HE1	1:A:440:TRP:CD2	2.57	0.40
3:b:23:ARG:HH22	3:b:580:HIS:C	2.30	0.40
3:b:64:MET:HB3	3:b:64:MET:HE2	1.79	0.40
3:b:411:MET:HE2	3:b:411:MET:HB3	1.94	0.40
1:A:488:HIS:O	1:A:489:HIS:HB2	2.22	0.40
1:A:659:GLN:HE21	1:A:659:GLN:HB2	1.71	0.40
2:B:328:THR:HG21	2:B:344:GLN:CB	2.50	0.40
2:B:493:PRO:HA	2:B:494:ALA:HA	1.36	0.40
3:b:57:ALA:O	3:b:60:ALA:HB3	2.21	0.40
3:b:86:LEU:HD23	3:b:142:CYS:HB2	2.03	0.40
3:b:269:ASP:HB3	3:b:424:LEU:HD13	2.04	0.40
4:C:14:ASP:O	4:C:18:GLU:N	2.55	0.40
3:b:97:TYR:HE1	3:b:146:ALA:HB2	1.86	0.40
3:b:182:MET:CE	3:b:198:ASN:HB2	2.52	0.40
3:b:362:TYR:CD1	3:b:597:ARG:HG2	2.56	0.40

All (1) 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)
1:A:199:ARG:NH1	1:A:684:ALA:O[10_665]	2.07	0.13

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

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	559/560 (100%)	504 (90%)	55 (10%)	7	25
2	B	588/604 (97%)	538 (92%)	50 (8%)	10	31
3	b	504/511 (99%)	439 (87%)	65 (13%)	4	13
4	C	115/116 (99%)	94 (82%)	21 (18%)	2	6
All	All	1766/1791 (99%)	1575 (89%)	191 (11%)	6	21

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	67	LEU
1	A	78	VAL
1	A	90	ILE
1	A	151	GLU
1	A	178	ARG
1	A	185	LEU
1	A	186	ARG
1	A	198	LEU
1	A	202	SER
1	A	204	ILE
1	A	206	VAL
1	A	213	THR
1	A	220	THR
1	A	223	ILE
1	A	235	THR
1	A	255	GLN
1	A	277	VAL
1	A	292	LEU
1	A	304	SER
1	A	311	GLN
1	A	325	LEU
1	A	345	LYS
1	A	347	THR

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Mol	Chain	Res	Type
1	A	371	VAL
1	A	381	SER
1	A	388	SER
1	A	400	VAL
1	A	409	SER
1	A	427	ARG
1	A	429	THR
1	A	442	VAL
1	A	445	ARG
1	A	460	VAL
1	A	479	VAL
1	A	503	LYS
1	A	518	THR
1	A	529	ILE
1	A	531	GLU
1	A	537	SER
1	A	540	ILE
1	A	552	THR
1	A	553	ILE
1	A	566	VAL
1	A	580	SER
1	A	601	LEU
1	A	605	VAL
1	A	608	GLU
1	A	632	SER
1	A	634	LEU
1	A	655	GLU
1	A	657	LEU
1	A	665	ILE
1	A	677	VAL
1	A	683	ARG
2	B	8	ASP
2	B	10	ILE
2	B	37	CYS
2	B	46	ILE
2	B	49	LEU
2	B	64	GLU
2	B	67	LEU
2	B	84	LEU
2	B	104	ILE
2	B	121	ARG
2	B	128	ASN

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Mol	Chain	Res	Type
2	B	135	GLU
2	B	137	ASP
2	B	142	VAL
2	B	205	HIS
2	B	206	ILE
2	B	237	GLN
2	B	244	ILE
2	B	248	TRP
2	B	262	MET
2	B	265	ASN
2	B	318	LEU
2	B	328	THR
2	B	350	SER
2	B	432	GLU
2	B	434	ILE
2	B	453	LYS
2	B	459	ARG
2	B	471	PHE
2	B	477	THR
2	B	491	VAL
2	B	505	ILE
2	B	530	VAL
2	B	549	GLU
2	B	558	ASP
2	B	574	VAL
2	B	584	LEU
2	B	587	ARG
2	B	590	GLU
2	B	597	GLN
2	B	600	GLU
2	B	604	SER
2	B	614	LYS
2	B	631	THR
2	B	636	ILE
2	B	638	GLU
2	B	675	LEU
2	B	696	VAL
2	B	702	LEU
2	B	713	GLU
3	b	1	MET
3	b	11	THR
3	b	26	ILE

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Mol	Chain	Res	Type
3	b	31	THR
3	b	68	SER
3	b	72	THR
3	b	73	THR
3	b	82	SER
3	b	88	VAL
3	b	89	THR
3	b	93	GLU
3	b	94	GLU
3	b	100	VAL
3	b	159	LYS
3	b	170	ILE
3	b	174	VAL
3	b	185	LEU
3	b	186	ARG
3	b	203	THR
3	b	235	VAL
3	b	241	THR
3	b	244	VAL
3	b	248	GLU
3	b	253	PHE
3	b	255	THR
3	b	267	LEU
3	b	271	VAL
3	b	280	THR
3	b	286	ARG
3	b	304	GLN
3	b	311	ARG
3	b	312	SER
3	b	314	VAL
3	b	315	VAL
3	b	328	VAL
3	b	377	VAL
3	b	394	VAL
3	b	411	MET
3	b	414	LEU
3	b	424	LEU
3	b	440	MET
3	b	462	VAL
3	b	470	ILE
3	b	483	LEU
3	b	489	VAL

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Mol	Chain	Res	Type
3	b	494	LEU
3	b	506	ARG
3	b	523	GLU
3	b	535	THR
3	b	542	GLN
3	b	546	SER
3	b	556	VAL
3	b	561	VAL
3	b	564	LEU
3	b	567	LEU
3	b	576	VAL
3	b	587	ASP
3	b	600	ARG
3	b	611	VAL
3	b	628	VAL
3	b	632	SER
3	b	633	THR
3	b	642	TRP
3	b	643	GLN
3	b	644	LEU
4	C	8	THR
4	C	16	ASN
4	C	25	CYS
4	C	27	THR
4	C	30	ILE
4	C	31	SER
4	C	42	VAL
4	C	44	GLU
4	C	45	ARG
4	C	46	ARG
4	C	75	CYS
4	C	79	THR
4	C	80	ARG
4	C	82	ILE
4	C	85	GLU
4	C	99	VAL
4	C	101	ILE
4	C	112	VAL
4	C	121	THR
4	C	124	GLU
4	C	127	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	127	GLN
1	A	255	GLN
1	A	274	GLN
1	A	311	GLN
1	A	397	ASN
1	A	404	GLN
1	A	562	GLN
1	A	612	GLN
2	B	111	GLN
2	B	282	ASN
2	B	457	HIS
2	B	575	ASN
3	b	74	ASN
3	b	187	HIS
3	b	193	HIS
3	b	202	HIS
3	b	304	GLN
3	b	492	GLN
3	b	580	HIS
4	C	81	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](#)

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 for Mogul analysis.

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
7	EPE	A	704	-	15,15,15	0.79	1 (6%)	19,20,20	1.76	5 (26%)
8	ADP	b	801	-	28,29,29	1.42	4 (14%)	43,45,45	1.92	7 (16%)
7	EPE	B	802	-	15,15,15	0.93	1 (6%)	19,20,20	2.01	6 (31%)
7	EPE	b	802	-	15,15,15	0.95	1 (6%)	19,20,20	1.82	4 (21%)

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
7	EPE	A	704	-	-	4/9/19/19	0/1/1/1
8	ADP	b	801	-	-	6/16/32/32	0/3/3/3
7	EPE	B	802	-	-	1/9/19/19	0/1/1/1
7	EPE	b	802	-	-	5/9/19/19	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	b	801	ADP	C5-C4	4.81	1.47	1.39
7	b	802	EPE	C10-S	3.29	1.82	1.77
7	B	802	EPE	C10-S	3.18	1.82	1.77
8	b	801	ADP	C5-C6	2.63	1.48	1.41
7	A	704	EPE	C10-S	2.57	1.81	1.77
8	b	801	ADP	C5-N7	-2.39	1.34	1.39
8	b	801	ADP	C8-N7	2.27	1.36	1.31

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	b	801	ADP	C5-C4-N3	-6.58	117.66	126.72
7	B	802	EPE	C5-N4-C3	5.36	120.39	108.84
8	b	801	ADP	N3-C4-N9	5.25	136.10	127.17
7	b	802	EPE	C5-N4-C3	4.60	118.75	108.84
8	b	801	ADP	C2-N3-C4	3.97	121.52	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	704	EPE	C5-N4-C3	3.68	116.77	108.84
7	B	802	EPE	C7-N4-C3	3.56	120.72	111.24
7	A	704	EPE	O3S-S-C10	3.47	112.80	106.00
7	b	802	EPE	C7-N4-C5	3.40	120.30	111.24
8	b	801	ADP	N3-C2-N1	-3.24	123.68	128.58
7	b	802	EPE	C7-N4-C3	3.20	119.76	111.24
8	b	801	ADP	C4-C5-N7	-3.18	106.94	110.58
7	A	704	EPE	C7-N4-C5	3.06	119.40	111.24
7	A	704	EPE	C7-N4-C3	2.97	119.16	111.24
7	B	802	EPE	O1S-S-C10	2.88	111.08	106.73
7	B	802	EPE	C5-C6-N1	-2.50	105.60	110.65
7	b	802	EPE	O3S-S-C10	2.45	110.79	106.00
8	b	801	ADP	C5-N7-C8	2.44	107.29	103.45
8	b	801	ADP	O4'-C1'-N9	2.30	112.51	108.09
7	B	802	EPE	C2-C3-N4	2.22	115.13	110.65
7	B	802	EPE	C7-N4-C5	2.15	116.97	111.24
7	A	704	EPE	C6-N1-C2	2.08	113.31	108.84

There are no chirality outliers.

All (16) torsion outliers are listed below:

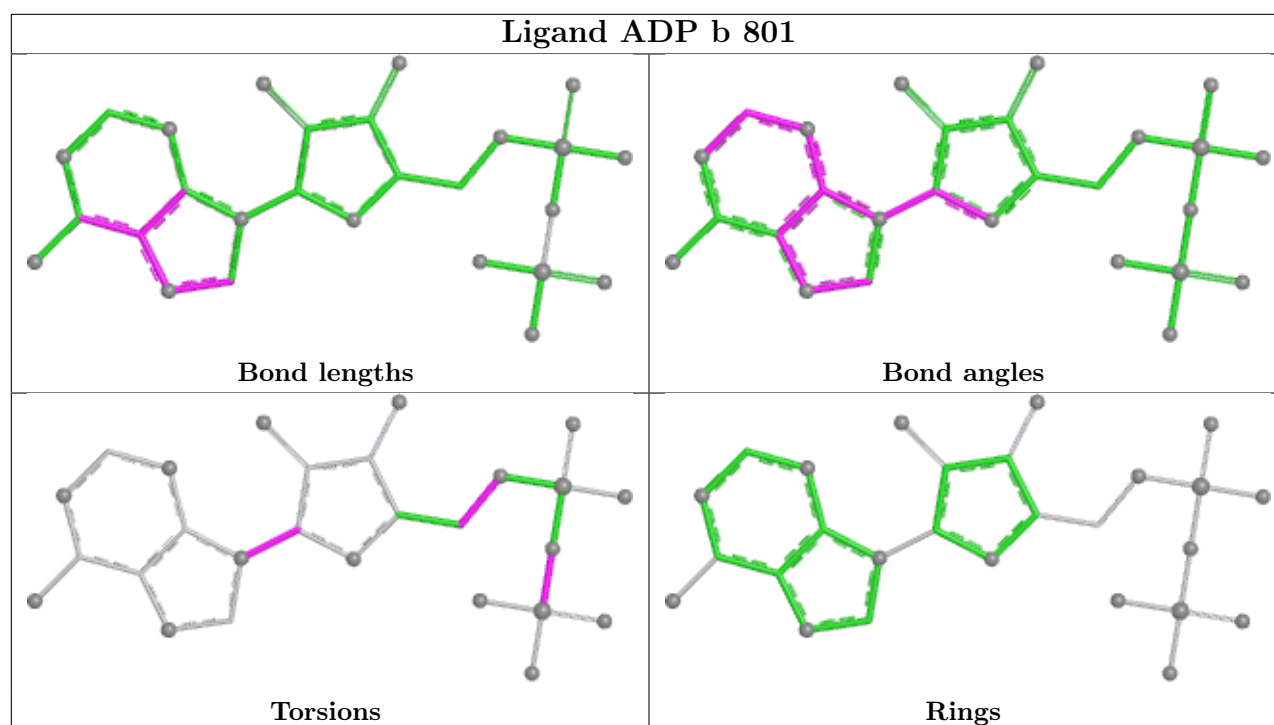
Mol	Chain	Res	Type	Atoms
7	A	704	EPE	S-C10-C9-N1
7	b	802	EPE	C10-C9-N1-C2
7	B	802	EPE	C8-C7-N4-C3
7	b	802	EPE	N4-C7-C8-O8
7	b	802	EPE	C8-C7-N4-C3
7	b	802	EPE	C8-C7-N4-C5
8	b	801	ADP	PA-O3A-PB-O1B
7	A	704	EPE	C10-C9-N1-C6
7	b	802	EPE	C10-C9-N1-C6
8	b	801	ADP	PA-O3A-PB-O2B
7	A	704	EPE	C8-C7-N4-C3
7	A	704	EPE	C10-C9-N1-C2
8	b	801	ADP	O4'-C1'-N9-C8
8	b	801	ADP	C4'-C5'-O5'-PA
8	b	801	ADP	C2'-C1'-N9-C4
8	b	801	ADP	C2'-C1'-N9-C8

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	704	EPE	1	0
8	b	801	ADP	2	0
7	b	802	EPE	2	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	683/684 (99%)	-0.57	4 (0%) 85 81	56, 85, 131, 191	0
2	B	711/732 (97%)	-0.47	11 (1%) 72 64	61, 92, 136, 224	0
3	b	649/658 (98%)	0.17	33 (5%) 33 26	81, 127, 202, 256	0
4	C	127/129 (98%)	-0.28	3 (2%) 59 50	94, 117, 142, 250	0
All	All	2170/2203 (98%)	-0.30	51 (2%) 59 50	56, 99, 179, 256	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	b	375	LEU	6.8
2	B	632	TRP	6.7
4	C	125	ALA	5.3
3	b	561	VAL	4.5
3	b	483	LEU	4.5
2	B	406	TYR	4.3
3	b	552	LEU	4.3
3	b	601	PHE	4.3
3	b	567	LEU	4.3
4	C	127	VAL	4.2
3	b	485	TRP	4.1
3	b	536	VAL	4.0
2	B	9	ALA	3.9
3	b	337	ALA	3.8
3	b	599	MET	3.7
3	b	540	LEU	3.6
3	b	550	ASP	3.6
2	B	633	LYS	3.3
2	B	385	GLY	3.3
4	C	1	MET	3.1
1	A	58	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
3	b	339	PRO	3.0
3	b	396	LEU	2.9
3	b	535	THR	2.7
3	b	481	VAL	2.6
3	b	639	PRO	2.6
3	b	533	VAL	2.6
1	A	621	ALA	2.6
2	B	718	ALA	2.5
3	b	531	ALA	2.5
3	b	404	ARG	2.5
2	B	635	PRO	2.5
3	b	400	ALA	2.5
3	b	345	GLY	2.4
3	b	556	VAL	2.4
2	B	8	ASP	2.3
3	b	564	LEU	2.3
2	B	329	PHE	2.3
3	b	398	VAL	2.2
3	b	149	PHE	2.2
3	b	641	ARG	2.2
3	b	642	TRP	2.2
3	b	362	TYR	2.2
3	b	600	ARG	2.2
2	B	118	VAL	2.1
1	A	2	ALA	2.1
3	b	545	ALA	2.1
3	b	1	MET	2.0
1	A	255	GLN	2.0
2	B	122	ARG	2.0
3	b	582	MET	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](#)

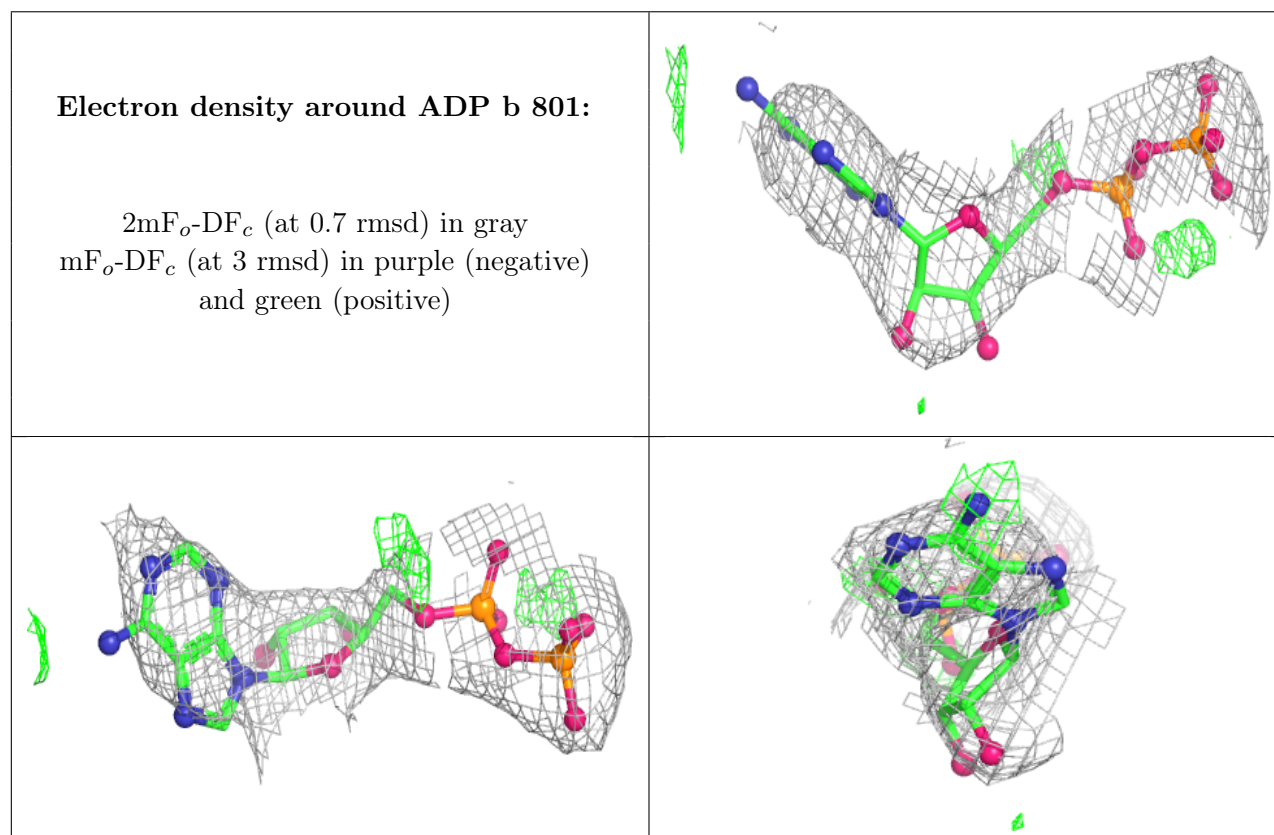
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
5	HG	B	801	1/1	0.73	0.14	200,200,200,200	1
7	EPE	b	802	15/15	0.86	0.15	137,142,148,151	0
8	ADP	b	801	27/27	0.90	0.12	147,169,177,180	0
7	EPE	A	704	15/15	0.91	0.13	109,129,136,136	0
6	K	A	703	1/1	0.94	0.19	103,103,103,103	0
5	HG	A	702	1/1	0.94	0.12	192,192,192,192	1
7	EPE	B	802	15/15	0.97	0.10	95,104,116,120	0
5	HG	C	201	1/1	0.99	0.05	247,247,247,247	1
5	HG	A	701	1/1	0.99	0.06	118,118,118,118	1

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.