Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 10:10 PM EDT

PDB ID	:	5L9W
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 (i) 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 (i)) were used in the production of this report:

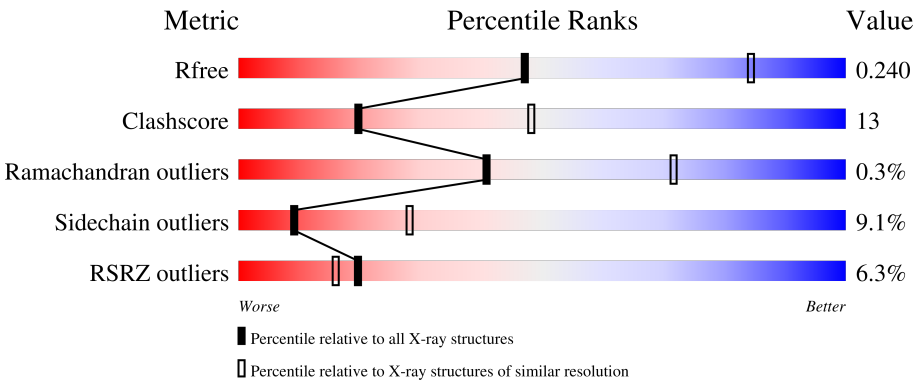
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 <=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	6% 72% 25% •
2	B	732	2% 68% 26% • •
3	b	658	12% 89% 9% •
4	C	129	5% 64% 32% • •

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	683	5285	3336	910	1002	37	0	0	0

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

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

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

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

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

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

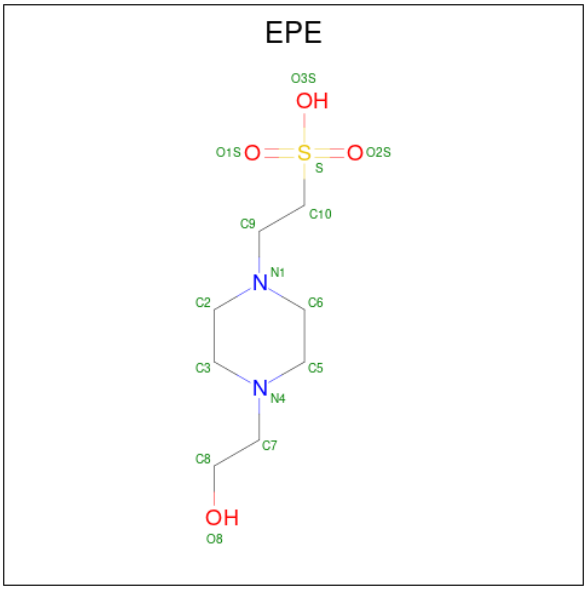
- Molecule 5 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

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

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

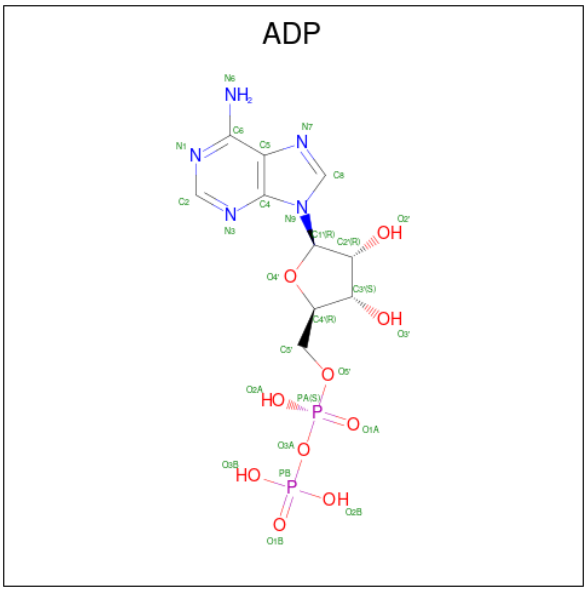
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
6	A	1	1	1	0	0

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



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

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



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

- Molecule 9 is water.

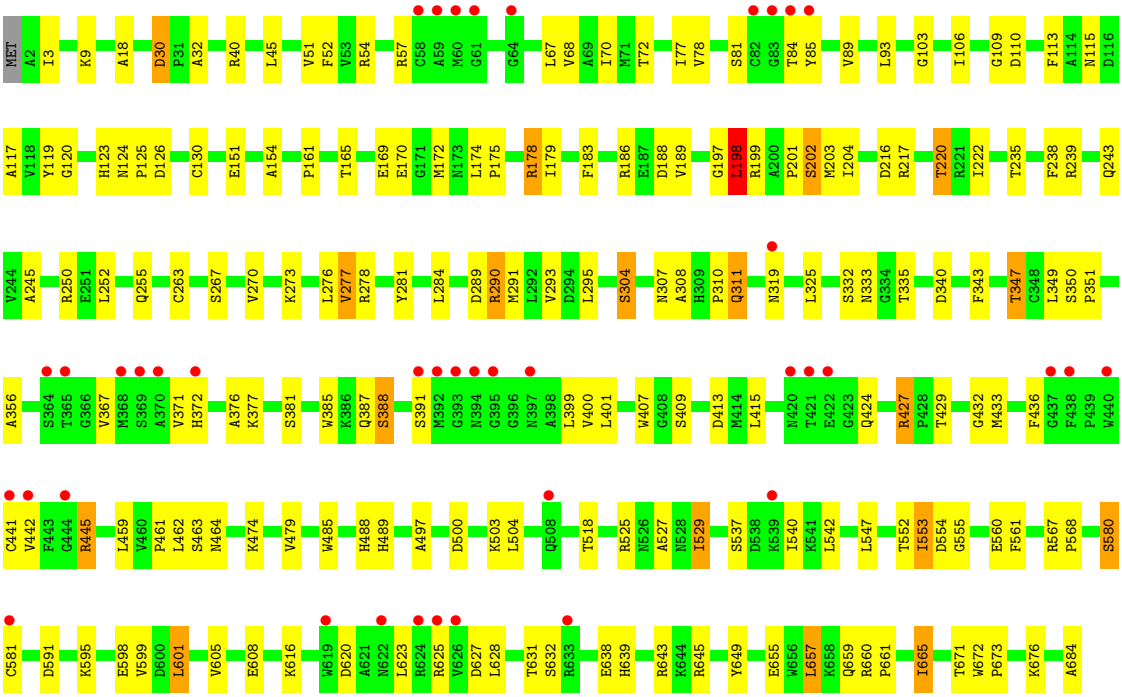
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	8	8	8	0	0
			Total	O		
9	B	6	6	6	0	0

3 Residue-property plots (i)

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.

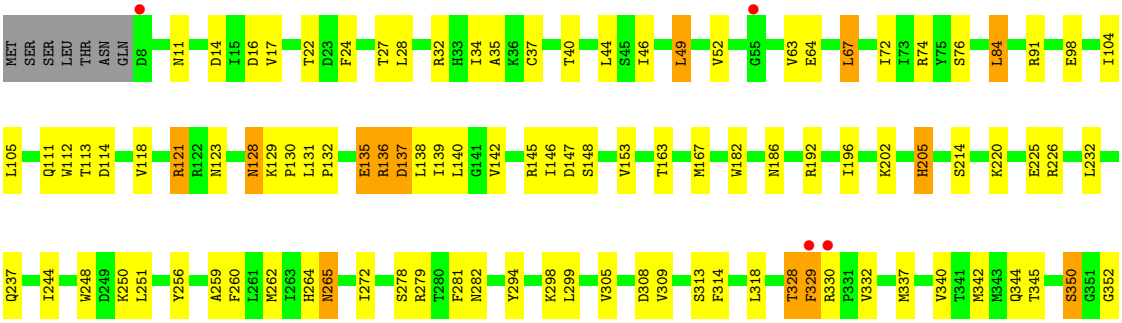
- Molecule 1: Acetophenone carboxylase delta subunit

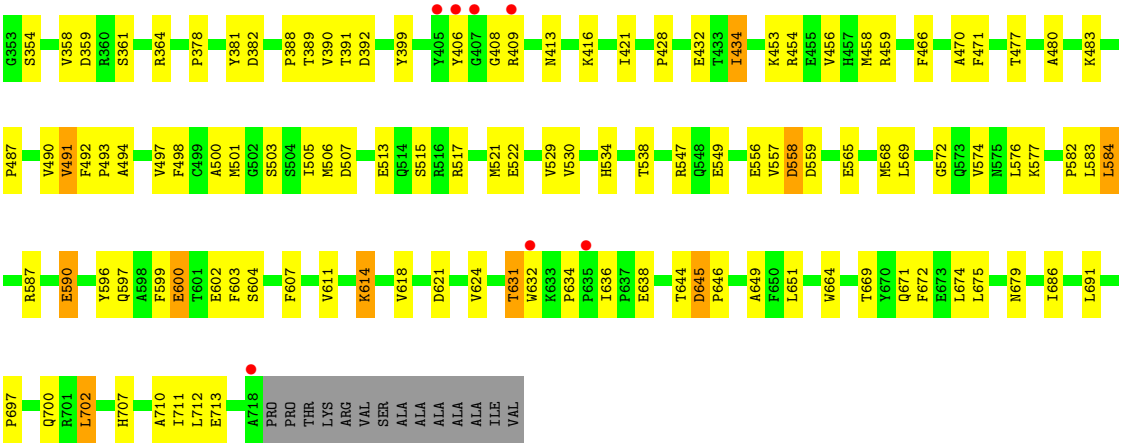
Chain A:



- Molecule 2: Acetophenone carboxylase gamma subunit

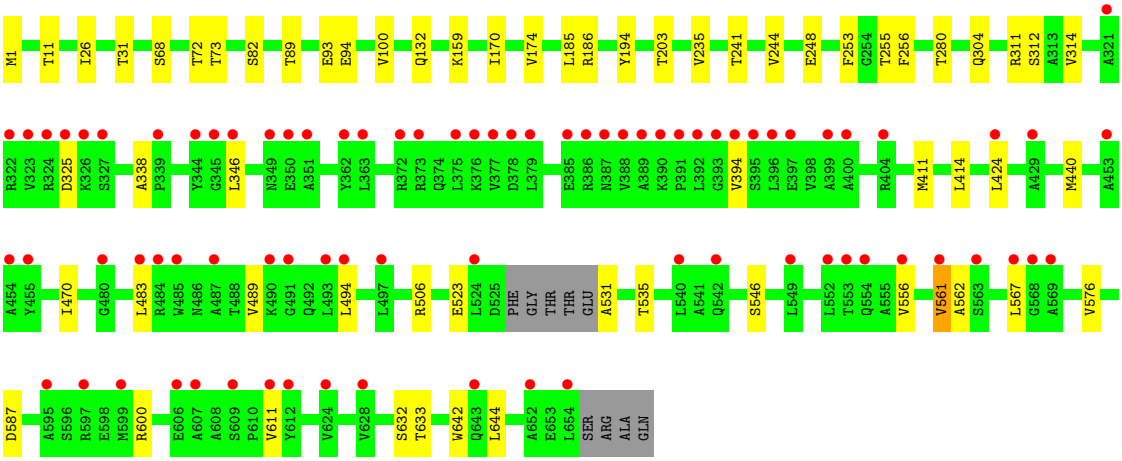
Chain B:





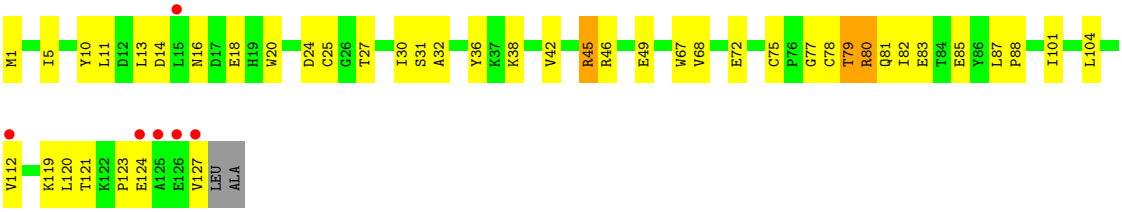
• Molecule 3: Acetophenone carboxylase alpha subunit

Chain b:



• Molecule 4: Acetophenone carboxylase beta subunit

Chain C:



4 Data and refinement statistics (i)

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 49.37 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.4 (19.97-2.90) 94.2 (49.37-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.197 , 0.235 0.201 , 0.240	Depositor DCC
R_{free} test set	6616 reflections (5.02%)	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)	0.33 , 83.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

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

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	0.48	1/5408 (0.0%)	0.67	2/7340 (0.0%)
2	B	0.45	1/5622 (0.0%)	0.64	0/7627
3	b	0.38	0/4925	0.61	0/6693
4	C	0.37	0/1067	0.56	0/1446
All	All	0.44	2/17022 (0.0%)	0.64	2/23106 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	CYS	CB-SG	-5.60	1.72	1.81
2	B	590	GLU	CG-CD	5.21	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	601	LEU	CA-CB-CG	7.85	133.35	115.30
1	A	126	ASP	CB-CG-OD2	6.29	123.96	118.30

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	115	1
2	B	5504	0	5495	132	0
3	b	4840	0	4829	0	0
4	C	1041	0	1017	27	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	1	0
7	b	15	0	17	0	0
8	b	27	0	12	0	0
9	A	8	0	0	0	0
9	B	6	0	0	0	0
All	All	16761	0	16564	257	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 (257) 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)
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
1:A:525:ARG:NH2	1:A:568:PRO:O	2.18	0.77
1:A:377:LYS:NZ	4:C:83:GLU:OE2	2.20	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
2:B:503:SER:HA	2:B:506:MET:HE2	1.79	0.64
1:A:179:ILE:HB	1:A:189:VAL:HG11	1.80	0.64
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:328:THR:HG21	2:B:344:GLN:HB3	1.82	0.61
1:A:347:THR:HG23	1:A:349:LEU:H	1.64	0.61
1:A:367:VAL:O	1:A:371:VAL:HG23	2.01	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
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
1:A:239:ARG:O	1:A:243:GLN:HG3	2.02	0.60
2:B:111:GLN:HG2	2:B:129:LYS:HD3	1.84	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
2:B:702:LEU:HD21	2:B:710:ALA:HB1	1.83	0.59
1:A:385:TRP:CD1	4:C:119:LYS:HE3	2.36	0.59
2:B:534:HIS:O	2:B:538:THR:HG23	2.03	0.59
2:B:131:LEU:HD12	2:B:132:PRO:HD2	1.86	0.58
2:B:24:PHE:HB3	2:B:35:ALA:HB3	1.86	0.58
1:A:527:ALA:HB1	1:A:553:ILE:HD11	1.85	0.58
2:B:406:TYR:C	2:B:408:GLY:H	2.07	0.57
1:A:347:THR:HG22	1:A:350:SER:OG	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
2:B:163:THR:O	2:B:167:MET:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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
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
2:B:521:MET:HE3	2:B:614:LYS:O	2.08	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
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
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
2:B:359:ASP:HB2	2:B:364:ARG:H	1.73	0.52
4:C:30:ILE:HD11	4:C:38:LYS:C	2.30	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
4:C:104:LEU:HD11	4:C:120:LEU:HD11	1.91	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
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
2:B:632:TRP:C	2:B:634:PRO:HD3	2.30	0.51
1:A:276:LEU:HD21	4:C:88:PRO:HB3	1.92	0.51
2:B:378:PRO:HD2	2:B:381:TYR:CD1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:ASP:HB3	2:B:153:VAL:HG21	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
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
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
2:B:105:LEU:HD11	2:B:136:ARG:HB2	1.93	0.49
2:B:40:THR:HG21	2:B:46:ILE:HG22	1.95	0.49
1:A:103:GLY:HA2	1:A:106:ILE:HD12	1.94	0.49
2:B:406:TYR:O	2:B:408:GLY:N	2.45	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
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
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
1:A:459:LEU:O	1:A:461:PRO:HD3	2.14	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
1:A:445:ARG:HH22	2:B:114:ASP:CG	2.17	0.47
2:B:568:MET:HB2	2:B:599:PHE:CE1	2.48	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
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
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: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
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
1:A:119:TYR:CE1	1:A:175:PRO:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:340:VAL:O	2:B:342:MET:HG3	2.15	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
2:B:358:VAL:HG11	2:B:428:PRO:HB2	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
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
1:A:433:MET:SD	2:B:128:ASN:HA	2.56	0.46
2:B:265:ASN:ND2	2:B:279:ARG:HA	2.31	0.46
1:A:660:ARG:HG2	1:A:661:PRO:O	2.16	0.45
2:B:521:MET:HE2	2:B:618:VAL:HG23	1.97	0.45
1:A:57:ARG:HH21	1:A:413:ASP:CG	2.20	0.45
2:B:697:PRO:HD2	2:B:700:GLN:HG3	1.99	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
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
2:B:492:PHE:CD2	2:B:498:PHE:HD1	2.33	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
1:A:40:ARG:HD2	1:A:40:ARG:HA	1.74	0.44
2:B:558:ASP:N	2:B:558:ASP:OD1	2.49	0.44
1:A:84:THR:HB	1:A:441:CYS:SG	2.58	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:CG	2:B:256:TYR:HB2	2.47	0.44
2:B:67:LEU:HD21	2:B:251:LEU:HD23	1.99	0.44
1:A:293:VAL:HG12	1:A:295:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:57:ARG:NH2	1:A:413:ASP:OD2	2.49	0.44
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
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
2:B:454:ARG:O	2:B:458:MET:HG3	2.18	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
2:B:329:PHE:CG	2:B:330:ARG:N	2.87	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
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
2:B:503:SER:HA	2:B:506:MET:CE	2.47	0.43
1:A:620:ASP:OD2	1:A:623:LEU:HD13	2.19	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
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
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
2:B:244:ILE:HG13	2:B:272:ILE:HD11	2.02	0.42
4:C:5:ILE:HB	4:C:13:LEU:HB3	2.01	0.42
1:A:560:GLU:CD	1:A:567:ARG:HH12	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:9:LYS:HG2	1:A:93:LEU:HD13	2.01	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
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
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
2:B:84:LEU:HD11	2:B:232:LEU:HD22	2.02	0.41
7:B:802:EPE:H21	7:B:802:EPE:H102	3.06	0.41
2:B:565:GLU:HB2	2:B:624:VAL:HB	2.01	0.41
2:B:308:ASP:O	2:B:314:PHE:HA	2.20	0.41
2:B:359:ASP:OD2	2:B:361:SER:N	2.41	0.41
1:A:643:ARG:NH2	4:C:77:GLY:H	2.14	0.41
1:A:616:LYS:O	1:A:631:THR:HG23	2.21	0.41
2:B:309:VAL:HG22	2:B:314:PHE:CD1	2.55	0.41
2:B:497:VAL:O	2:B:500:ALA:HB3	2.20	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
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:298:LYS:HE2	2:B:707:HIS:NE2	2.36	0.41
2:B:521:MET:CE	2:B:618:VAL:HG23	2.51	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
2:B:454:ARG:HG2	2:B:458:MET:CE	2.51	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:C:14:ASP:O	4:C:18:GLU:N	2.55	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 (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	681/684 (100%)	636 (93%)	44 (6%)	1 (0%)	51	82
2	B	709/732 (97%)	665 (94%)	41 (6%)	3 (0%)	34	66
3	b	645/658 (98%)	598 (93%)	45 (7%)	2 (0%)	41	71
4	C	125/129 (97%)	119 (95%)	6 (5%)	0	100	100
All	All	2160/2203 (98%)	2018 (93%)	136 (6%)	6 (0%)	41	71

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	b	561	VAL
3	b	338	ALA
1	A	198	LEU
2	B	136	ARG
2	B	329	PHE
2	B	645	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	559/560 (100%)	516 (92%)	43 (8%)	13	35
2	B	588/604 (97%)	544 (92%)	44 (8%)	13	37
3	b	504/511 (99%)	446 (88%)	58 (12%)	5	17
4	C	115/116 (99%)	99 (86%)	16 (14%)	3	10
All	All	1766/1791 (99%)	1605 (91%)	161 (9%)	9	28

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	30	ASP
1	A	52	PHE
1	A	67	LEU
1	A	78	VAL
1	A	151	GLU
1	A	178	ARG
1	A	198	LEU
1	A	202	SER
1	A	204	ILE
1	A	220	THR
1	A	235	THR
1	A	255	GLN
1	A	263	CYS
1	A	277	VAL
1	A	290	ARG
1	A	304	SER
1	A	311	GLN
1	A	325	LEU
1	A	347	THR
1	A	381	SER
1	A	388	SER
1	A	409	SER
1	A	427	ARG

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Mol	Chain	Res	Type
1	A	429	THR
1	A	436	PHE
1	A	442	VAL
1	A	445	ARG
1	A	479	VAL
1	A	518	THR
1	A	529	ILE
1	A	537	SER
1	A	540	ILE
1	A	553	ILE
1	A	561	PHE
1	A	580	SER
1	A	601	LEU
1	A	605	VAL
1	A	608	GLU
1	A	632	SER
1	A	655	GLU
1	A	657	LEU
1	A	665	ILE
2	B	37	CYS
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
2	B	135	GLU
2	B	137	ASP
2	B	142	VAL
2	B	145	ARG
2	B	205	HIS
2	B	237	GLN
2	B	248	TRP
2	B	260	PHE
2	B	262	MET
2	B	264	HIS
2	B	265	ASN
2	B	328	THR
2	B	350	SER
2	B	382	ASP
2	B	432	GLU

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Mol	Chain	Res	Type
2	B	434	ILE
2	B	453	LYS
2	B	459	ARG
2	B	477	THR
2	B	491	VAL
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	702	LEU
2	B	713	GLU
3	b	1	MET
3	b	11	THR
3	b	26	ILE
3	b	31	THR
3	b	68	SER
3	b	72	THR
3	b	73	THR
3	b	82	SER
3	b	89	THR
3	b	93	GLU
3	b	94	GLU
3	b	100	VAL
3	b	132	GLN
3	b	159	LYS
3	b	170	ILE
3	b	174	VAL
3	b	185	LEU
3	b	186	ARG
3	b	194	TYR
3	b	203	THR
3	b	235	VAL

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Mol	Chain	Res	Type
3	b	241	THR
3	b	244	VAL
3	b	248	GLU
3	b	253	PHE
3	b	255	THR
3	b	256	PHE
3	b	280	THR
3	b	304	GLN
3	b	311	ARG
3	b	312	SER
3	b	314	VAL
3	b	325	ASP
3	b	346	LEU
3	b	394	VAL
3	b	411	MET
3	b	414	LEU
3	b	424	LEU
3	b	440	MET
3	b	470	ILE
3	b	483	LEU
3	b	489	VAL
3	b	494	LEU
3	b	506	ARG
3	b	523	GLU
3	b	535	THR
3	b	546	SER
3	b	556	VAL
3	b	561	VAL
3	b	567	LEU
3	b	576	VAL
3	b	587	ASP
3	b	600	ARG
3	b	611	VAL
3	b	632	SER
3	b	633	THR
3	b	642	TRP
3	b	644	LEU
4	C	1	MET
4	C	16	ASN
4	C	25	CYS
4	C	27	THR
4	C	31	SER

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Mol	Chain	Res	Type
4	C	42	VAL
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	101	ILE
4	C	112	VAL
4	C	121	THR
4	C	127	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	255	GLN
1	A	274	GLN
1	A	311	GLN
1	A	404	GLN
1	A	612	GLN
2	B	128	ASN
2	B	282	ASN
2	B	457	HIS
3	b	74	ASN
3	b	187	HIS
3	b	193	HIS
3	b	202	HIS
3	b	304	GLN
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 monosaccharides 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	b	802	-	15,15,15	0.95	1 (6%)	18,20,20	1.93	4 (22%)
7	EPE	B	802	-	15,15,15	0.93	1 (6%)	18,20,20	2.11	7 (38%)
7	EPE	A	704	-	15,15,15	0.79	1 (6%)	18,20,20	1.92	4 (22%)
8	ADP	b	801	-	24,29,29	1.00	2 (8%)	29,45,45	1.45	4 (13%)

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	b	802	-	-	5/9/19/19	0/1/1/1
7	EPE	B	802	-	-	1/9/19/19	0/1/1/1
7	EPE	A	704	-	-	4/9/19/19	0/1/1/1
8	ADP	b	801	-	-	4/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	b	802	EPE	C10-S	3.30	1.82	1.77
7	B	802	EPE	C10-S	3.19	1.82	1.77
7	A	704	EPE	C10-S	2.59	1.81	1.77
8	b	801	ADP	C5-C4	2.55	1.47	1.40
8	b	801	ADP	O4'-C1'	2.16	1.44	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	802	EPE	C5-N4-C3	5.14	120.39	108.83
7	b	802	EPE	C5-N4-C3	4.41	118.75	108.83
7	A	704	EPE	O3S-S-C10	4.35	112.80	105.77
8	b	801	ADP	PA-O3A-PB	-3.83	119.70	132.83
7	B	802	EPE	C7-N4-C3	3.71	120.72	111.23
7	b	802	EPE	C7-N4-C5	3.54	120.30	111.23
7	A	704	EPE	C5-N4-C3	3.53	116.77	108.83
7	B	802	EPE	O1S-S-C10	3.46	111.08	106.92
7	b	802	EPE	C7-N4-C3	3.33	119.76	111.23
8	b	801	ADP	N3-C2-N1	-3.20	123.68	128.68
7	A	704	EPE	C7-N4-C5	3.19	119.40	111.23
7	b	802	EPE	O3S-S-C10	3.10	110.79	105.77
7	A	704	EPE	C7-N4-C3	3.10	119.16	111.23
8	b	801	ADP	C3'-C2'-C1'	2.81	105.20	100.98
7	B	802	EPE	C5-C6-N1	-2.46	105.60	110.64
8	b	801	ADP	C4-C5-N7	-2.36	106.94	109.40
7	B	802	EPE	C7-N4-C5	2.24	116.97	111.23
7	B	802	EPE	O2S-S-C10	2.21	109.58	106.92
7	B	802	EPE	C2-C3-N4	2.19	115.13	110.64

There are no chirality outliers.

All (14) torsion outliers are listed below:

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

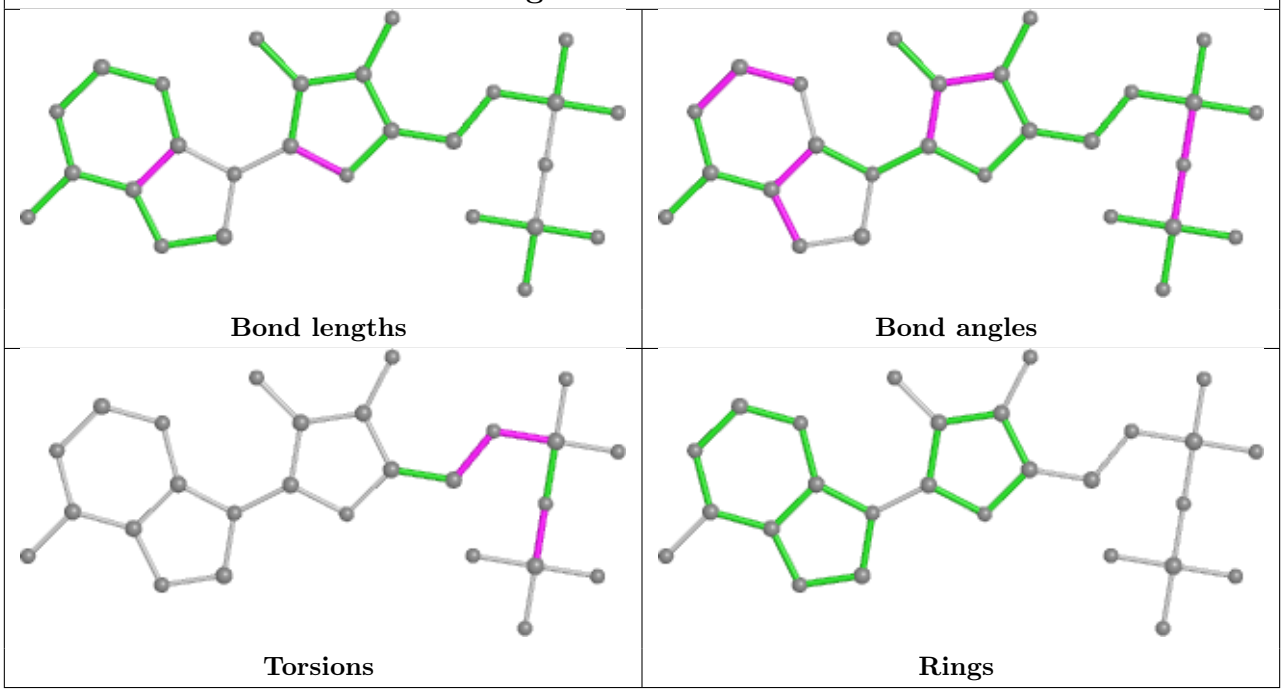
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	802	EPE	1	0
7	A	704	EPE	1	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 then 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.

Ligand ADP b 801



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	683/684 (99%)	0.26	40 (5%)	22	18	56, 85, 131, 191	0
2	B	711/732 (97%)	-0.07	11 (1%)	73	73	61, 92, 136, 224	0
3	b	649/658 (98%)	0.46	80 (12%)	4	3	81, 127, 202, 256	0
4	C	127/129 (98%)	0.26	6 (4%)	31	28	94, 117, 142, 250	0
All	All	2170/2203 (98%)	0.21	137 (6%)	20	16	56, 99, 179, 256	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	C	127	VAL	8.9
3	b	485	TRP	6.3
4	C	125	ALA	6.3
3	b	339	PRO	6.2
3	b	490	LYS	6.0
1	A	58	CYS	5.9
2	B	407	GLY	5.5
2	B	632	TRP	5.4
3	b	345	GLY	5.1
3	b	569	ALA	5.1
2	B	406	TYR	5.0
1	A	441	CYS	5.0
1	A	624	ARG	5.0
3	b	540	LEU	4.8
3	b	568	GLY	4.4
1	A	626	VAL	4.4
3	b	321	ALA	4.4
2	B	8	ASP	4.4
3	b	484	ARG	4.2
3	b	599	MET	4.0
3	b	556	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
3	b	385	GLU	3.9
3	b	391	PRO	3.9
3	b	324	ARG	3.9
2	B	329	PHE	3.9
3	b	393	GLY	3.8
3	b	453	ALA	3.8
3	b	325	ASP	3.8
3	b	494	LEU	3.8
3	b	375	LEU	3.8
3	b	497	LEU	3.8
3	b	606	GLU	3.8
1	A	619	TRP	3.7
3	b	597	ARG	3.6
4	C	126	GLU	3.6
3	b	388	VAL	3.4
3	b	491	GLY	3.4
1	A	440	TRP	3.3
1	A	59	ALA	3.3
3	b	654	LEU	3.3
4	C	15	LEU	3.2
3	b	323	VAL	3.2
1	A	64	GLY	3.2
1	A	625	ARG	3.2
1	A	82	CYS	3.1
3	b	372	ARG	3.1
3	b	561	VAL	3.1
1	A	437	GLY	3.1
3	b	387	ASN	3.1
3	b	351	ALA	3.0
3	b	542	GLN	3.0
1	A	420	ASN	3.0
1	A	61	GLY	3.0
3	b	377	VAL	3.0
3	b	524	LEU	3.0
3	b	373	ARG	3.0
3	b	379	LEU	3.0
3	b	483	LEU	2.9
3	b	378	ASP	2.9
1	A	84	THR	2.9
3	b	349	ASN	2.9
3	b	397	GLU	2.8
2	B	409	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	393	GLY	2.8
4	C	112	VAL	2.8
1	A	622	ASN	2.8
3	b	487	ALA	2.8
1	A	395	GLY	2.7
3	b	326	LYS	2.7
1	A	391	SER	2.7
3	b	394	VAL	2.7
3	b	424	LEU	2.7
2	B	635	PRO	2.7
3	b	493	LEU	2.7
3	b	350	GLU	2.7
3	b	454	ALA	2.7
1	A	369	SER	2.6
3	b	563	SER	2.6
1	A	581	CYS	2.6
3	b	392	LEU	2.6
1	A	368	MET	2.6
1	A	421	THR	2.6
1	A	394	ASN	2.6
3	b	612	TYR	2.6
1	A	422	GLU	2.6
3	b	552	LEU	2.5
3	b	376	LYS	2.5
3	b	607	ALA	2.5
3	b	344	TYR	2.5
3	b	643	GLN	2.5
3	b	390	LYS	2.5
1	A	83	GLY	2.4
3	b	624	VAL	2.4
3	b	628	VAL	2.4
1	A	319	ASN	2.4
3	b	400	ALA	2.4
3	b	595	ALA	2.4
3	b	609	SER	2.4
3	b	346	LEU	2.4
3	b	567	LEU	2.4
3	b	389	ALA	2.3
1	A	539	LYS	2.3
3	b	386	ARG	2.3
3	b	553	THR	2.3
1	A	60	MET	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	405	TYR	2.3
1	A	365	THR	2.3
3	b	611	VAL	2.3
2	B	718	ALA	2.2
4	C	124	GLU	2.2
3	b	322	ARG	2.2
1	A	372	HIS	2.2
1	A	438	PHE	2.2
3	b	455	TYR	2.2
3	b	396	LEU	2.2
1	A	364	SER	2.2
3	b	429	ALA	2.2
1	A	444	GLY	2.2
2	B	55	GLY	2.2
1	A	397	ASN	2.2
1	A	392	MET	2.2
3	b	395	SER	2.1
3	b	399	ALA	2.1
1	A	633	ARG	2.1
1	A	508	GLN	2.1
3	b	327	SER	2.1
1	A	85	TYR	2.1
3	b	362	TYR	2.0
1	A	442	VAL	2.0
3	b	652	ALA	2.0
3	b	363	LEU	2.0
2	B	330	ARG	2.0
3	b	549	LEU	2.0
1	A	370	ALA	2.0
3	b	480	GLY	2.0
3	b	404	ARG	2.0
3	b	554	GLN	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 monosaccharides in this entry.

6.4 Ligands (i)

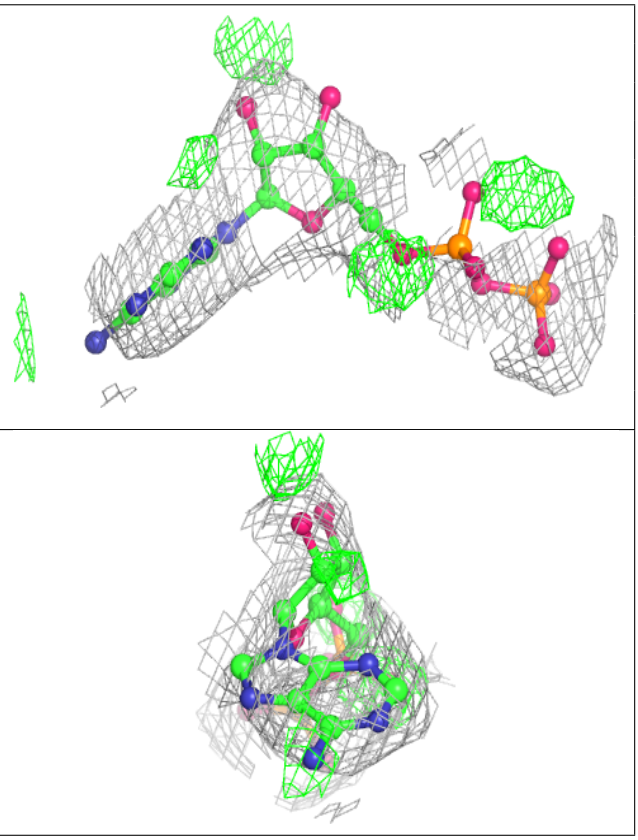
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	HG	B	801	1/1	0.61	0.12	200,200,200,200	1
7	EPE	b	802	15/15	0.90	0.30	137,142,148,151	0
8	ADP	b	801	27/27	0.90	0.27	147,169,177,180	0
7	EPE	A	704	15/15	0.93	0.23	109,129,136,136	0
6	K	A	703	1/1	0.94	0.58	103,103,103,103	0
5	HG	A	702	1/1	0.95	0.50	192,192,192,192	1
7	EPE	B	802	15/15	0.97	0.15	95,104,116,120	0
5	HG	C	201	1/1	0.99	0.12	247,247,247,247	1
5	HG	A	701	1/1	0.99	0.23	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.

Electron density around ADP b 801:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.